REPUBLIC OF TURKEY

YILDIZ TECHNICAL UNIVERSITY

GRADUATE SCHOOL OF SCIENCE AND ENGINEERING

DESALINATION PERFORMANCE OF A CAPACITIVE DEIONIZATION CELL OPTIMIZED WITH ANSYS FLOW SIMULATION

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Mansoor Safwan Mansoor Mohammed AL-AGHBARI

Signature

The student thanks the Prime Ministry Presidency for Turks Abroad and Related Communities for their financial support.

Dedicated to my family

And my wife

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LIST OF SYMBOLS

V_c	High Potential Limit
I	Instant Current
V_a	Low Potential Limit
υ	Scan Rate
C_{cv}	Specific Capacitance
V	Volt

LIST OF ABBREVIATIONS

AC	Activated Carbon
ACC	Activated Carbon Cloth
BOD	Biological Oxygen Demand
CA	Carbon Aerogel
CB	Carbon Black
CD	Direct Current
CDI	Capacitive Deionization
CE	Counter Electrode
CFD	Computational Flow Dynamics
CNT	Carbon Nanotubes
COD	Chemical Oxygen Demands
CV	Cyclic Voltammetry
CVD	Chemical Vapor Deposition
DI	Deionized
ED	Electrodialysis
EDL	Electrical Double Layer
FDM	Fused Deposition Modeling
GHG	Green House Gas
GR	Graphene
HFC	Hexagonal Flow Channel
MED	Multi Effect Distillation
MESNT	Multi-walled Carbon Nanotube
MSF	Multi-Stage Flash Distillation
NMP	N-Methyl-2-Pyrrolidone
OMC	Ordered Mesoporous Carbon
PANI	Polyaniline
PFC	Perfect Square Flow Channel
PLA	Poly Lactic Acid
PPy	polypyrrole
PTFE	Polytetrafluoroethylene
PVDF	Polyvinylidene Fluoride

RO	Reverse Osmosis
SA	Surface Area
SAC	Salt Adsorption Capacity
SWCNT	Single-walled Carbon Nanotube
TDS	Total Dissolved Solids
USGS	United States Geological Survey
WRI	World Resources Institute
WE	Working Electrode

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ABSTRACT

Desalination Performance of A Capacitive Deionization Cell Optimized With Ansys Flow Simulation

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Department of Chemical Engineering

Master of Science Thesis

Supervisor: Assoc. Prof. Dr. Dilek DURANOĞLU

Water purification is a fundamental process for the sustainability of water resources. Therefore, the development of water treatment technologies in terms of low energy consumption and high salt removal capacity is highly important. Capacitive deionization (CDI) is a new water treatment method that might be utilized efficiently in desalination purposes. It can be used to produce purified, potable water by removing ions from seawater and brackish water. Here we utilized computational fluid dynamics (CFD) using ANSYS 21 (student version) software to introduce an optimized design for capacitive deionization (CDI) cell. The design focused on producing uniform flow over the electrode area in order to enhance the surface utilization of electrodes. After 3D printing of developed CDI cell, desalination performance of capacitive deionization process was investigated by using 2mM NaCl in a batch system. Optimum operation parameters like potential, flow rate and time were determined. Maximum salt adsorption capacity of 2.9 mg/g was obtained at 1.2 V potential, 20 mL/min flow rate and 15 min adsorption/desorption period. The optimized CDI cell design enhanced the salt

adsorption capacity of the process by 47%. The electrodes exhibited a stable performance and full regeneration over long adsorption/desorption cycles.

Keywords: Desalination, capacitive deionization, flow simulation, ANSYS.

ÖZET

Ansys Flow Simülasyonu İle Optimize Edilmiş Kapasitif Deiyonizasyon Hücresinin Desalinasyon Performansi

Mansoor Safwan Mansoor Mohammed AL-AGHBARI

Kimya Mühendisliği Anabilim Dalı

Yüksek Lisans Tezi

Danışman: Doç.Dr. Dilek DURANOĞLU

Su arıtma, su kaynaklarının sürdürülebilirliği için temel bir süreçtir. Bu nedenle, düşük enerji tüketimi ve yüksek tuz giderme kapasitesi açısından su arıtma teknolojilerinin geliştirilmesi oldukça önemlidir. Kapasitif deiyonizasyon (KDI), desalinasyon amacıyla verimli bir şekilde kullanılabilen yeni bir su arıtma yöntemidir. Deniz suyundan ve acı sudan iyonları uzaklaştırarak arıtılmış, içilebilir su üretmek için kullanılabilir. Bu çalışmada, kapasitif deiyonizasyon (KDI) hücresinin optimum tasarımı hesaplamalı akışkan dinamiği (CFD) kullanılarak ANSYS 21 (öğrenci versiyonu) akış simülasyonu ile gerçekleştirilmiştir. Tasarım sırasında elektrotların yararlanımını arttırmak için elektrotların yüzeyinde homojen bir akış sağlanmasına odaklanılmıştır. Geliştirilen KDI hücresinin üç boyutlu baskısından sonra, kesikli bir sistemde 2mM NaCl kullanılarak kapasitif deiyonizasyon prosesinin desalinasyon performansı incelenmiştir. Optimum çalışma parametreleri (potansiyel farkı, akış hızı ve süre) belirlenmiştir. 1,2 V potansiyel farkı, 20 mL/dak akış hızı ve 15 dakikalık adsorpsiyon/desorpsiyon süresinde 2,9 mg/g desalinasyon kapasitesi elde edilmiştir. Optimize edilen CDI hücre tasarımı, elektrotun tuz adsorpsiyon kapasitesini %47 artırmıştır. Ayrıca

elektrotlar, uzun adsorpsiyon/desorpsiyon döngüleri boyunca kararlı bir performans ve tam rejenerasyon sergilemiştir.

Anahtar Kelimeler: Desalinasyon, kapasitif deiyonizasyon, akış simülasyonu, ANSYS.

1
INTRODUCTION

One of the 21st-century concern is the accessibility of clean and affordable water. Demand of freshwater resources has been increasing as a result of population growth, economic development, urbanization, modern industry, growing agricultural practices, and global warming (Yasin et al., 2016; Rasines et al., 2015).

Nowadays, a wide range of technologies, for example, membrane processes (including electrodialysis (ED), reverse osmosis (RO), and nanofiltration), as well as thermal processes like multi-stage flash distillation (MSF) and multi-effect distillation (MED), are employed for softening and desalination applications. The current trend in desalination is to use the RO process followed by MED and MSF processes (Gude, 2016; Wang et al. 2015). While thermal and membrane desalination systems provide excellent deionization, their key drawbacks are their secondary pollutant creation and high energy requirements, resulting in a high operational/maintenance cost. It has become critical to create more energy-efficient, environmentally friendly, and cost-effective methods for sea/brackish water desalination (Wang et al., 2015; Eke et al., 2020).

Capacitive deionization (CDI) is a revolutionary method of water treatment that might be utilized efficiently in desalination. Capacitive deionization (CDI) technique is a unique, electrochemically regulated desorption/sorption method that helps to remove charged ions like; hardness, salt, arsenic, heavy metals, and other ions from various water types (Welgemoed & Schutte, 2005; García-Quismondo et al., 2013). The water to be desalinated is routed inside a cell consists of an electrode couple. These electrodes are constructed of porous conductive materials and fitted in the cell. In CDI, direct current is delivered to the cell. An electrosorption stage is conducted in which the ions present in the water to be treated are trapped into the electrical filed formed near electrodes surface, causing the ions to be extracted from the water. After a certain amount

of time, saturation of the electrodes will be reached, at which point the potential difference is disconnected or reversed to allow the ions to be released back into the concentrate flow and assist electrodes regeneration (Wang et al., 2015; Anderson et al., 2010). These discharge and charge electrowetting stages may be run in series or parallel to create concentrated brine and purified water, respectively.

In CDI process, the fundamental mechanism is the formation of electrical double layer (EDL). Applying electrical potential difference to electrodes causes cations and anions found in the solution to be attracted and trapped onto the electrical field near electrode with the help of Coulomb force (electrostatic forces), creating EDL. By getting the rid of the electrostatic forces, ions return to solution. This operating mechanism is utilized in the CDI process, as deionization and regeneration (Zhang & Zhao.,2009). Recently, in comparison to other deionization processes, CDI technology has gained increasing interest of researchers thanks to the advancements in technology of nanomaterials and potential of this technology to replace current desalination technologies (Wang et al., 2015; Porada et al., 2013).

In order to optimize the performance of the CDI process, three parameters must be considered; cell geometry like flow-by or flow-through, operation parameters like applied potential, flow rate, initial concentration, cycle time, and electrode materials like carbon-based, metal oxide, conducting polymer, conductive additives, polymer binders, and current collector (He et al., 2018). Many studies have been published aiming to optimize the desalination process. He et al. (2018), Alencherry et al. (2017), Chen et al. (2018) and Li et al. (2018) have investigated the effect of materials. Some of them have studied the effect of parameters like applied voltage range (Zhang et al., 2018), effluent concentration (Jande & Kim, 2013). Others have investigated the effect of CDI cell geometry to optimize the pressure drop, energy consumption (Laxman et al., 2019; Jeon et al., 2017; Lado et al., 2021). All optimization attempts aimed to increase the salt removal capacity with lower energy consumption.

There is an obvious need for CDI system design studies to reduce the magnitude and sources of resistive losses resulting from electrosorption and ion transport (Patel et al., 2020). The architectural design of CDI cell must consider features such as mass transport, flow distribution, long-term stability, current density distribution rates, and electrode potential distribution (Vlad et al., 2015; Newman, 1968).

The impact of fluid flow on pressure drop is critical for lowering energy usage and enhancing the ability of CDI cells to compete with more established technologies. The few previous works that have addressed this issue have focused on various aspects such as the adjustment of flow patterns in cells of various shapes (Jeon et al., 2017). Laxman et al. (2019) have taken it a step further by evaluating computational fluid dynamic (CFD) simulation of the pressure drop encountered by a fluid within single CDI cells with various designs They also emphasized the necessity of efficient fluid distribution in helping the scaling up and commercialization of CDI cells (Laxman et al.,2019). Taking this into account, here the design of flow frame distribution was investigated in order to ensure optimal performance of the system.

In this study, computational fluid dynamics (CFD) software ANSYS 21 (student version) was used to introduce an optimized design for capacitive deionization (CDI) cell. While designing the cell, producing uniform flow over the electrode area was prioritized in order to enhance the surface utilization of electrodes. After 3D printing of optimized CDI cell, optimum operation parameters – potential difference, concentration, flow rate and time- of capacitive deionization process was investigated and determined by using 2mM NaCl solution in a batch system.

1.1 Literature Review

Recent conducted studies on developing CDI processes have been summarized below.

Hou et al. (2012) studied the influence of adding polyvinylidene fluoride (PVDF) to activated carbon powder in the CDI process. Mixtures with a weight ratio of 10%, 20%, 30%, and 40% (PVDF) were used to prepare 4 electrodes with an area of 80 mm x 80 mm and thickness of 0.38 mm. The used AC has 1124 m^2/g specific

surface area. Galvanostatic and cyclic voltammetry (CV) experiments were carried out to analyze the electrochemical properties of the electrodes. The concentration of the solution used was 2mM NaCl. The charging and discharging voltages were 1.2 V and 0.0 V, respectively. The experimental results showed that the electrochemical stability and mechanical strength were good with increasing weight fraction of (PVDF). Conversely, the electrosorption capacity decreased as the (PVDF) content clogged the activated carbon pores and led to a decrease in the effective surface area. The electrode with 10 wt% (PVDF) exhibited sufficient mechanical and electrochemical stability. The electrosorption efficiency was 96.7% and the electrosorption capacity was 44.5 mmol/g. (Hou et al., 2012).

Jeon et al. (2017) investigated the effect of flow pattern on CDI cell. The investigation was carried out by performing CFD simulation to hexagonal flow channel (HFC) and perfect square flow channel (PFC) cells. The analysis aimed to minimize the dead zones of the empirical design of PFC. Then, several comparison tests were carried out to see the effect of adjustments made to the empirical design. CFD results showed that PFC design had larger dead zones than the HFC design. They claimed that by decreasing the dead zones in the cell the salt adsorption capacity increased. The CDI experiments results confirmed the claims as the adsorption capacity was greater in HFC than in PFC. Also, they investigated the effect of concentration, flow rate and time. They stated that the longer the time, the more adsorbed ions before saturation reached. Also, the higher the voltage, the greater the adsorption capacity. They showed that higher flow rates decreased residence time and resulted with lower the capacity of the system (Jeon et al., 2017).

Alencherry et al., (2017) studied the use of powdered activated carbon impregnated with silver to investigate the role of hydrophilicity and electrical conductivity on the electrode electrosorption capacity for capacitive deionization. In the study, three types of electrodes were fabricated over a graphite sheet in a disc form with a 7.5 cm diameter 1.35 mm thickness. The electrode active material mass was 9.5 (± 0.3) g. The first electrode composition was powdered activated carbon, polyethylene binder, and carbon black in the 70:20:10 ratio. The second electrode was made with the same composition as the first but with 0.2% silver-

impregnated powder activated carbon (AgPAC). As the third one, a functionalized multi-walled carbon nanotube (MWCNT) was added to the mixture of the second electrode in the 1:99 ratio with AgPAC. 10mL of 600 ppm NaCl solution was used. The applied DC voltage was 1.2 V. A 16min-charge/discharge cycles were performed. The silver content in the second electrode increased electrosorption capacity from 2 to 5.3 mg/g. The hydrophilicity of the electrodes was increased as a result of MWCNT addition which improved the salt removal kinetics and enhanced the salt removal up to 60% as well (Alencherry et al., 2017).

Laxman et al., (2019) developed a CFD model to optimize and study the distribution of fluid velocity in order to minimize the pressure losses of the fluid. Also, they have constructed CDI cell to verify the predicted models. The pressure drop, fluid flow parameters and salt adsorption capacity were obtained experimentally as well. They showed that by decreasing the path traveled by the fluid and fluid velocity the pressure drops decreases. The experimental results showed a 60% of pressure drops and 35% increase of the salt adsorption capacity. They stated that higher SAC and lower pressure drop can be achieved by modifying the input and output part of the cell (Laxman et al., 2019).

Ji et al., (2019) reported a novel design for high-performance CDI with nano-porous carbon film electrodes that are free-standing and highly compact using activated microporous carbon particles (PPy-AMC) derived from polypyrrole with 5% polymer binder. Three different electrodes prepared with different activated carbons were used for comparison purposes. Precisely, AC -1, AC -2, and PACMM. Exchange membranes with 0.140 mm and 0.170 mm thickness for anions and cations, respectively. The total mass of the electrodes for AC -1, AC -2, and PACMM were 0.16 g, 0.28 g, 0.30 g, and 1.37 g, respectively. The size of each electrode was 4x4 cm^2. 20 mM NaCl was supplied to the cell from a 10-liter tank using a peristaltic pump at a rate of 10 mL/min for constant voltage operation and 4 mL/min for the constant current operation. Constant voltage operation was performed with three charge-discharge cycles of 2400 s each. In the discharge step, 0 V was applied, while in the charge step, a range from 0.4 V to 1.2 V was applied. For constant current operation, 1.5 V was applied during charging with different current densities, and 0 V was applied during discharging. The study has

demonstrated that PPy-AMC exhibited the highest equilibrium salt adsorption capacity compared to commercial CDI electrodes due to its high surface area of about 2800 m^2/g and particle distribution of nearly 240 nm (Ji et al., 2019).

Hack et al. (2019) have demonstrated CDI systems can be used for biotechnology. They have used CDI cells to concentrate crotonic acid. They built a lab-scale model. The used electrodes were made of activated carbon. The mixture of the electrode was 10% polyvinylidene fluoride (PVDF), 85% activated carbon Norit SX ultra, and 5% carbon black. Rapid prototyping technique was utilized to create the cell chamber and the ladder-like spacer used to isolate the electrodes, using the acrylate-based 3D printing materials VeroClear and VeroWhitePlus. Figure 1.1 shows the image of the 3D manufactured CDI cell. Liquid phase enters through the top lid and flows via a thin gap between the working electrode (WE) and counter electrode (CE) until it reaches a transversely arrayed exit located in the bottom lid. A ladder-like spacer is used to separate the electrodes and titanium clamps are used to connect the electrodes to the potentiostat. The electrodes were able to adsorb approximately 0.1 mmol of crotonic acid per gram of electrode material when 1.2 V was applied, and the feed solution was adjusted to a pH of 7. The estimated energy consumption of such a system is around 1 kWh for $1m^3/h$ of a 20 mM crotonic acid feed (Hack et al., 2019).

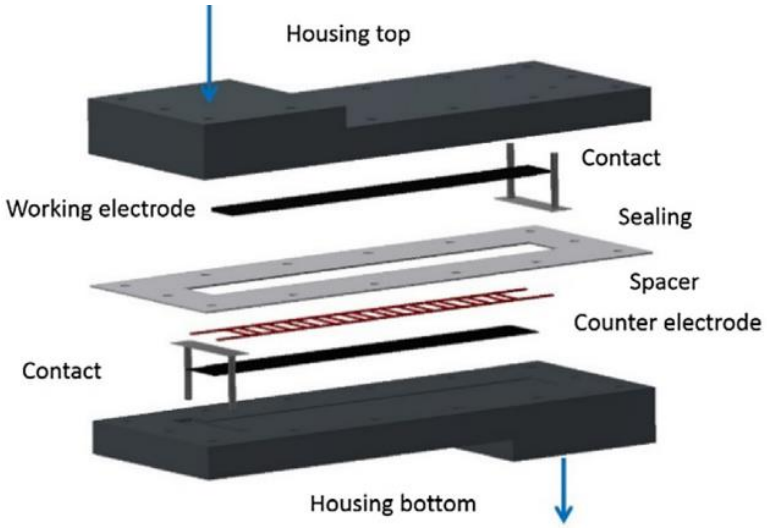


Figure 1.1 3D printed CDI cell (Hack et al., 2019)

Zhang et al. (2019) utilized carbon aerogels with varying porous structure as electrodes in a CDI application to eliminate ions from a salt solution. The current collector is 10x10 cm^2 in size. The electrodes had a working surface of 6 x 6 cm^2. The CDI components fundamental structure is comprised of a row of plates that support the other components (Figure. 1.2). The support plate is constructed entirely of organic glass represented as (. 1) in Figure 1.2 In order to prevent leakage, rubber gaskets were utilized (2). The electrodes (3) were separated by a 5 mm gap using spacer (4). Cells were 100 x 100 x 12.2 mm^3 in total. The final salt adsorption capacity of the carbon aerogel electrode was 25.45 mg/g (Zhang et al., 2019).

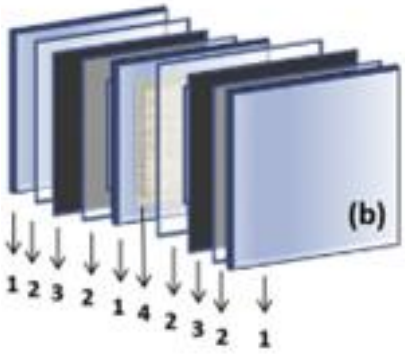


Figure 1.2 Clarification of the CDI unit utilized (Zhang et al., 2019)

Folaranmi et al., (2020) synthesized an electrode from activated carbon and graphene oxide for brackish water desalination. In the study, activated carbon and graphite powder, carbon black, and graphite foil (0.35 mm thick) was used. As binder, Polyvinylidene fluoride (PVDF) was used. The mixture of activated carbon was mixed with graphene oxide in different weight ratios and cast into 6 x 10 cm^2 graphite flakes. The CDI system was operated in batch mode and consisted of a peristaltic pump, a CDI cell, a DC power source (Potentiostat) and a conductivity meter. The electrodes in the CDI cell were separated by an insulator (0.99 mm thick). The brine concentration was 400 mg/L and 1200 mg/L NaCl and was supplied at a rate of 25 mL/min at room temperature. The applied potential differences were 1.0 V and 1.4 V. The electrodes containing 15 wt.% graphene oxide exhibited the highest salt adsorption capacity of (5.70 mg/g) among the other electrodes, with a capacitance of 75 F/g and average salt adsorption rate of

0.34 mg/g/min. This enhancement was due to the fact that the addition of graphene oxide increased the hydrophilicity of the electrode surface, thus improving the interaction between the salt ions and electrode surface (Folaranmi et al., 2020).

Lado et al., (2021) has characterized a prototype of CDI equipped with 3D graphite felt electrodes utilizing a CFD simulation. The simulation was aimed to study the effect of including some small cavities in the inlet or perforated channels to achieve a uniform fluid flow distribution. After that they investigate the performance of the cell through CDI experiments with different operation parameters. The results showed that single pass operation produced larger amount of water than batch system but with lower salt concentration reduction. They emphasized on the balance between flow rate and current distribution as they both effect water production. Also, they reported that high flow rates lead to high production of water and lower salt concentration reduction (Lado et al., 2021).

1.2 Objective of the Thesis

The need for creating more energy efficient, environmentally friendly, and cost-effective methods for sea/brackish water desalination is crucial. Capacitive deionization (CDI) processes are one of the most promising method for this purposes. In this work, it was aimed to develop an optimum CDI cell design with ANSYS flow simulation that satisfy the following:

- Uniform fluid velocity profile over the electrodes to enhance the salt adsorption capacity.
- Low pressure drop across the CDI cell to decrease energy consumed by the pump
- Ease of production for scaling up the process

After developing optimum CDI cell, examination of desalination performance of CDI is another objective of this study.

1.3 Hypothesis

- Fluid flow regime is effective on the electrosorption kinetic due to the mass transfer limitations overall the electrodes. Accordingly CDI cell can be designed to obtain homogenous flow distribution with relatively high fluid flow.
- Decreasing the sharp corners in the transitions inlet and outlet will decrease the dead zones and pressure drop generated by expansion and comparison effect.
- Curving the wall will decrease the contact between the fluid and the wall that will decrease the friction and the distances needed to have homogenous velocity profile.
- These modifications can decrease the pressure drop, provide a uniform velocity profile, and enhance the salt adsorption capacity of the electrodes. Flow regime of the designed CDI cells can be investigated and optimized by using ANSYS flow simulation software.
- Optimized unique CDI cell can be manufactured easily by using a 3D printer, then desalination performance can be investigated experimentally.

2
GENEREAL INFORMATION

2.1 Global Challenge of Fresh Water

The demand for freshwater resources is continuously increasing as a result of population growth, economic development, urbanization, modern industry, growing agricultural practices, and global warming. (Yasin et al., 2016; Rasines et al., 2015).

One billion people or more worldwide do not have access to clean water since there are not enough water resources for agricultural and economic development in 36 nations. 33 nations, including Turkey, would have extremely high levels of water stress in 2040, so perhaps leaving these countries more susceptible to water scarcity than they already are at the present time. Given the rise in water consumption across the globe and the limited availability of suitable resources of freshwater, new, sustainable, and environmentally friendly water resources must be found (Maddocks et al., 2022).

United States Geological Survey (USGS) data indicate that over 97% of the Earth's natural water resources are brackish water and seawater, which are completely unsuited for irrigation, residential, industrial, hydroelectricity, or human consumption (Manju & Sagar, 2017). Nearly all the usable freshwater is in groundwater (49.3%), and glaciers (68.7%). Fresh water, with only 0.24% of the overall water supply, makes up the rest of the planet's water supply (Manju & Sagar, 2017). According to their salinity, water bodies are grouped as in Table 2.1.

Table 2.1 Classification of water salinity (Roy & Chowdhury, 2020)

Classification	Total Dissolved Solids (ppm)
Non-saline	<500
Slightly saline	500-1500
Moderately saline	1500-7000
Highly saline	7000-15000
Very Highly saline	15000-35000
Braine	>40000

With the notable exception of fresh water, the world's supply of water is far more brackish or saline than freshwater. Desalination is by far the most effective, reliable, and lasting way to obtain fresh water in these days. Seawater desalination is used to provide fresh water in areas where a shortage of water is particularly acute, such as Singapore and the Middle East (Manju & Sagar, (2017). Turkey currently faces water shortage, with each person getting only 1.519 m^3 of water per year in 2015, which is anticipated to be 1.120 m^3 by 2030. This essentially means that in the next years, Turkey will be facing a severe water shortage, and it will become a "water-poor" country (Uyduranoğlu Öktem & Aksoy, 2014).

Another method of obtaining fresh water is reusing and reclaiming industrial and municipal wastewater. Certain sectors, such as beverage and food, chemical, petroleum, textile tanning and leather tanning, cooling towers of power plants, produce effluent that has a high level of salt in it. While conventional methods of wastewater treatment are capable of removing nutrients (N, P) and organic matters from wastewater, the treated effluent retains dissolved salt. As a consequence of this, extra treatment of the treated effluent is required in order to remove salts from it before it can be recycled as useful recovered water (Lefebvre & Moletta, 2006). Desalination should therefore be viewed as a critical procedure for developing alternate supplies of fresh water.

Reclaimed water, because of its high salt content, has severe challenges. Salinity of water used for irrigation in agricultural and urban settings leads to the buildup

of ions such as sodium, calcium, magnesium, and others in the soil. Salinity in buildings causes soap anions to react with Ca^{+2} and Mg^{+2}, which results in a reduced cleaning effectiveness, and an increased laundry detergent usage. In addition, these ions produce scaling difficulties in heat exchangers, boilers, and electrical appliances and corrosions, which have a negative impact on the service life of these equipment (Zou et al., 2008). The risks associated with TDS levels in water are kept to a minimum by restricting their use in distinct areas, as seen in Table 2.2.

Table 2.2 Total dissolved solid limitations for water application

Usage		TDS limit (ppm)	Ref
Urban		< 2000	(EPA, 2012)
Agriculture		< 2000	
Industrial	Steam	0.5-1.0	
	Boiler	0.05 – 3500	
Drinking		< 600	(WHO, 2017)

2.2 Conventional Desalination Technologies

Wide range of technologies, for example, membrane processes (including electrodialysis (ED), reverse osmosis (RO), and nanofiltration), as well as thermal processes like: (multi-effect distillation (MED) and multi-stage flash distillation (MFD)), are employed for softening and desalination applications. Approximately two thirds of the world's population desalination capacity in the early 2000s was controlled by thermal methods. Now the focus has switched to processes that take place on the membrane since 2000. The current trend in desalination is to use the RO process followed by MED and MSF processes (Gude, 2016; Wang et al., 2015). Global desalination by used technology and by users can be seen in Figure 2.1. The largest share of the total world desalination capacity comes from seawater desalination at roughly 60%, this is then after that brackish water, which accounts for 21%, river , lake water, which accounts for 8%, and wastewater, which accounts for 6% (Gude, 2016).

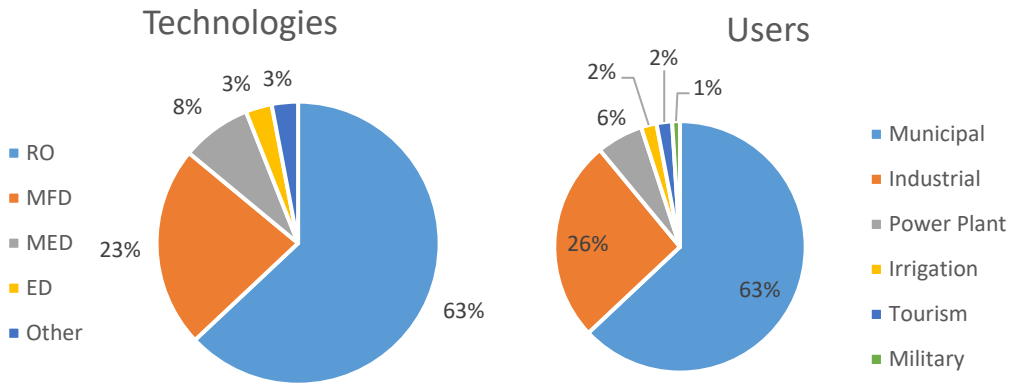


Figure 2.1 Desalination industry share by users and by technology (Gude, 2016)

As the demand for freshwater increases, the amount of available desalination capacity is rising steadily. Global desalination capacity increased 58 million m^3/day in 2008, followed by an increase of 74.8 million m^3/day in 2012. Then by 97.2 million m^3/day in 2020. In 2015, there were about 18,000 desalination plants with a treatment capacity of 86.8 million m^3 of water per day installed worldwide. Thousands of people in over 150 nations get fresh water from these plants (Eke et al., 2020).

While thermal and membrane desalination systems provide excellent deionization, their key drawbacks are secondary pollutant creation and high energy requirements, resulting in a high operational/maintenance cost. Conventional desalination processes remove ions from water effectively through the use of high-pressure membranes and high temperatures. Because the majority of present industrial scale desalination facilities are powered by fossil fuel combustion, this trade-off between emissions of CO_2 and production of freshwater increases global warming and has the potential to lead to a shortage of the latter. These techniques also include the use of treatment chemicals, which can be harmful to both aquatic and terrestrial ecosystems. As a result of these factors, it has become critical to create more energy-efficient, environmentally friendly, and

cost-effective methods for sea/brackish water desalination (Wang et al., 2015; Eke et al., 2020).

Capacitive deionization (CDI) is a revolutionary method of water treatment that can be utilized efficiently for desalination. This electrochemical deionization technique leverages the technology of supercapacitor electrodes in order to remove ions from water in an effective and ecologically friendly manner. Researchers have taken a keener interest in CDI technology in recent years than they have in other deionization procedures because of the potential it has to replace existing desalination methods and the advances made in nanomaterials technology (Porada et al., 2013; Wang et al., 2015).

2.3 Capacitive Deionization

Capacitive deionization (CDI) technique is a unique, electrochemically regulated adsorption/desorption method that helps to remove charged ions like; hardness, salt, arsenic, heavy metals, and other ions from various water types (Welgemoed & Schutte, 2005; García-Quismondo et al., 2013). The schematic explanation of a CDI process can be seen in Figure 2.2. The water to be desalinated is routed inside a cell made off with couples of electrodes. These electrodes are constructed of porous conductive materials and fitted in the cell. In CDI, direct current is delivered to the cell. An electrosorption stage is conducted in which the ions present in the water are trapped into the electrical filed formed near electrodes surface, causing the ions to be extracted from the water. After a certain amount of time, saturation of the electrodes will be reached, at which point the applied potential is disconnected or reversed to allow the ions to be released back into the flow and assist electrodes regeneration. These discharge and charge electrowetting stages may be run in series or parallel to create concentrated brine and purified water, respectively. (Wang et al., 2015; Anderson et al., 2010).

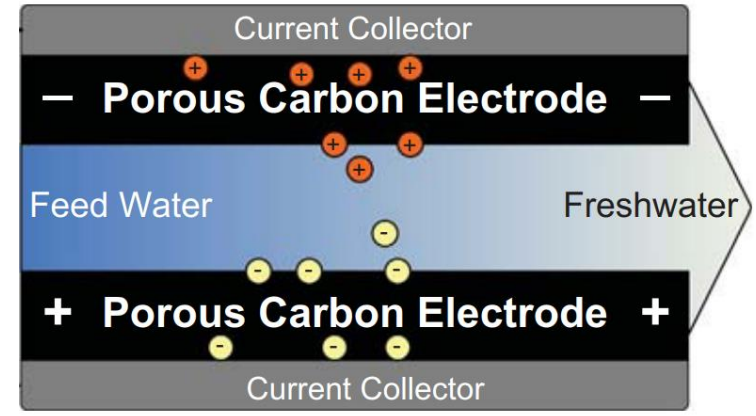


Figure 2.2 CDI Process (Porada et al., 2013)

2.3.1 Working Principles of CDI Process

In the CDI process, two basic methods are used for ion storage. EDL formation is the fundamental mechanism; applying electrical potential difference to electrodes causes cations and anions found in the solution to be attracted to and trapped onto the electrical filed near electrode with the help of Coulomb force (electrostatic forces), creating EDL. By removing the electrostatic forces, the ions return to the solution. This operating mechanism is utilized in the CDI process, as deionization and regeneration (Zhang & Zhao, 2009). Simplified EDL mechanism is illustrated in Figure 2.3. Double layer theory explains the interfacial characteristics and structure between an aqueous solution and electrode surface. This hypothesis says that the EDL is separated into two layers, which are called compact layer (Helmholtz layer) and diffuse layer (Gouy–Chapman layer). The total capacitance of the system is determined in part by the capacitance of both the diffuse and inner layer. The accumulation of electrostatic charge on the surface of carbon-derivatives is essential to the success of this approach. (Zhang & Zhao, 2009).

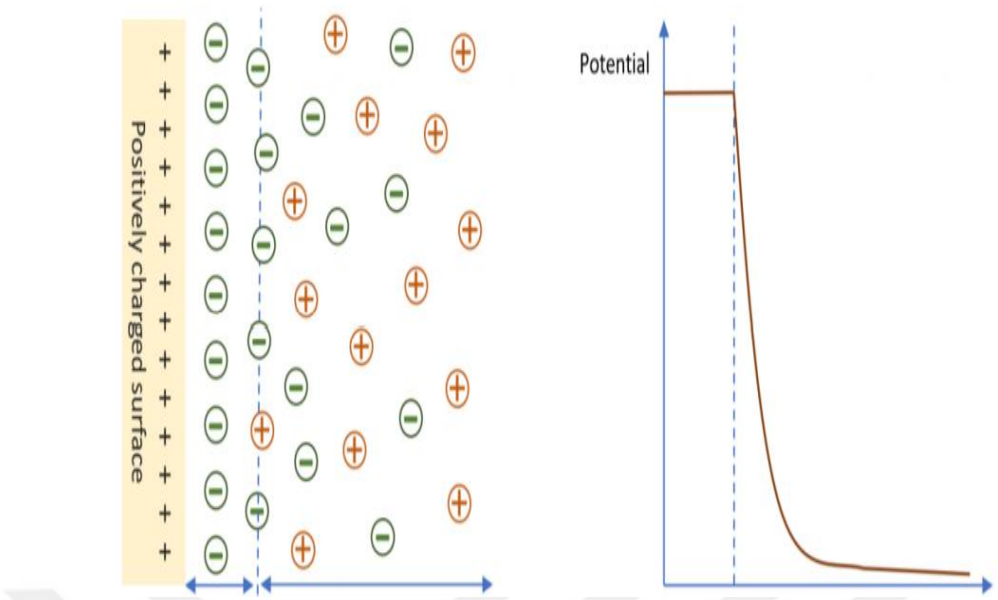


Figure 2.3 EDL and potential distribution (Porada et al., 2013)

While EDL mechanism stores ions only on the electrode surface. Faradaic charge transfer technique is also possible during CDI operation (pseudocapacitance). Faradaic mechanism stores the ions in the form of electron transfer between pseudocapacitive electrode materials and ions via rapid, reversible electrochemical reactions at the solution and electrode interface. Thus, it produces another mechanism that acts similarly to adsorption and desorption, which enables it to hold on to more ions on the surface of the electrode. Cation- and anion-selective pseudocapacitive electrode materials are the most typically researched in terms of linking anions and capturing cations (Zhang et al., 2018).

2.3.2 Advantages and Limitation of CDI Process

When compared to more traditional deionization methods, the CDI process has a variety of significant benefits that help solving both economic and environmental issues. In terms of energy efficiency, CDI is superior to other methods. Unlike membrane and thermal deionization processes, which require higher pressures and temperatures, CDI technology uses less energy. It can function at low voltage of between 1.2 and 2 volts and does not need high pressures or temperatures (Wang et al., 2015). Moreover, because it doesn't require an energy transformation, an advantage of CDI is that it must use electrical energy, rather than another source of energy.

It is feasible to recover a portion of the energy consumed using the CDI technology because of the use of electrodes that stores energy to deionize water. Some of the applied energy is released throughout the regeneration step, in which ions are discharged from the electrodes' surface. To charge another CDI unit, you can use this energy held in capacitors and utilize capacitive discharge coils to create the charge. Consequently, the CDI system can recover 50 - 70% of the energy it uses (Welgemoed & Schutte, 2005; Anderson et al., 2010). It is observed that the deionization process (CDI) utilizes far less energy (0.6 kWh/m^3) than other desalination procedures such as EDR (2.04 kWh/m^3) and RO (2.25 kWh/m^3), which are believed to be the most efficient currently available (Welgemoed & Schutte, 2005; Yu et al., 2016).

Conventional deionization processes, such as continuous use of chlorine species in the system, require an enormous amount of maintenance. This maintenance includes such tasks as frequent maintenance to prevent membrane fouling and scaling, which are dismissed into the environment as secondary pollutants in a disposal saltwater stream which can end up causing adverse effects on the environment. Precautionary measures should be taken prior to the release of these compounds into the environment (Wang et al., 2015). Thermal deionization techniques are also employed, resulting in higher water temperatures and possible pollution and disposal issues. Reduced oxygen solubility in water results in less oxygen being dissolved in water, which impairs aquatic ecosystems and increases the likelihood of deadly toxicity for immobilized and untreated species. Conversely, CDI procedures require less maintenance and produce fewer environmental and disposal risks (Welgemoed & Schutte, 2005).

The estimated cost of using Capacitive Deionization (CDI) technology for treating brackish water is lower than that of traditional methods, including capital, operation and maintenance expenses. The majority of the cost of CDI systems is made up of capital expenses. By developing more affordable nanomaterials for electrode preparation, the capital cost of CDI systems can be reduced, making it a more competitive option compared to conventional deionization processes for high-salinity brackish or seawater applications (Welgemoed & Schutte, 2005).

2.3.3 Electrode Materials Used in CDI Process

Because they have a key function in the electrosorption process, electrode materials are regarded as one of the highly important components of CDI processes. Nanostructured materials with outstanding properties have begun to be used frequently to create better supercapacitor electrodes as a result of recent material improvements. As a result, active electrodes surface area may be increased, and therefore the enhanced system efficiencies may be reached. To boost the water ion adsorption capacity, this field is merged with new research on the CDI technology (Porada et al., 2013).

Specific electrode characteristics must be employed in the supercapacitor electrodes of the CDI process to facilitate the removal of ions. Ions are stored at the electrode/solution interface, so ideal electrode materials should have large surface area that enhance the ions accessibility. Also, pore size should be ideal to allow the accumulation of higher number of ions with no additional limitations that can occur when ions diffuse or when kinetic factors are involved. Moreover, to keep energy dissipation and voltage drop to a minimum, materials should be conductive as higher as possible for minimizing the contact resistance between the current collector and the electrode. In addition, the wetting behavior (hydrophilicity) of the pores must be good, ensuring the whole volume of pore participation in the CDI process. Additionally, they should be electrochemically stable over the voltage and pH ranges in use. To ensure system endurance and prevent biofouling over time, they should also have strong bio-inertness (Oren, 2008).

Another significant consideration for the application of large-scale electrodes is that suitable electrode materials should possess a great natural abundance, scalable structure, and minimal carbon footprint. Although sustainability is affected by availability and environmental implications, it affects the price considerations as well. They should also be able to be processed and shaped into electrode sheets (Oren, 2008).

The following electrode materials are extensively utilized in CDI devices: carbon-based materials, conducting polymers, and metal oxides. By employing these

materials independently or as a nanocomposite, scientists can construct supercapacitor electrodes (Porada et al., 2013).

- Carbon-based materials

Carbon electrodes are frequently employed in supercapacitor electrodes due to their favorable characteristics. Specific surface area, conductivity, adjustable pore structure, and processability are the main characteristics needed to be as high as possible. Carbon materials' ion storage mechanism relies on using EDL on the electrode/solution interface to retain ions. Low contact resistance, chemical stability and, wetting behavior are some of the positive attributes of carbon-based electrodes. For these reasons, CDI often demonstrates high electrophoresis performance. The commonly used carbon-based nanomaterials in CDI process are carbon aerogel (CA), activated carbon (AC), ordered mesoporous carbon (OMC), graphene (GR) and carbon nanotube (CNT) (Wang et al., 2015; Ahmed & Tewari, 2018; Bai et al., 2014).

- Metal Oxides

Supercapacitor electrodes can also be made from metal oxides due to their pseudocapacitive characteristic. This is done by cathodic reduction, anodic oxidation, and faradaic ion storage, which takes place on the electrode surfaces and within the materials. However, as far as capacitance is concerned, metal oxides tend to have poor conductivity, but for theoretical capacitance, they are not bad. The other qualities metal oxides had (low cost, environmentally benign, natural abundance, and a simple means of anchoring them to the carbon structure) make them better candidates for the CDI applications (Oladunni et al., 2018).

- Conducting polymers

A pseudocapacitive substance utilized in supercapacitor electrodes is another type of conducting polymers. The Faradaic reduction/oxidation reactions employed in conducting polymers are comparable to metal oxides. Because of their general ability to provide specific capacitance, high conductivity when doped, inexpensive manufacturing costs, and high conductivity in the form of deposited particles, these electrodes are appropriate for most electrical applications (Oladunni et al., 22018; Thamilselvan et al., 2016).

- Conductive additives

To boost the electrical conductivity of CDI electrodes, conductive materials such as graphite powder and carbon black are often used. Studies have indicated that the primary factor affecting the efficiency of CDI process is the structure of pore and conductive additives (Nadakatti et al., 2011).

- Polymer binders

To give stable structure and to attach the electrode material to the current collector, polymeric binders are used in the preparation of CDI electrodes. Polyvinylidene fluoride (PVDF), Polytetrafluoroethylene (PTFE) are the most used frequent binders in CDI electrodes (Bian et al., 2013).

- Current collectors

A current collector is a substance that conducts electricity and serves as a connection surface for CDI electrodes. In a summary, the ideal current collector material should be resistive to corrosion and have electrochemical stability over the CDI system operating voltage range (Wang et al., 2012).

2.3.4 CDI Process Configuration

2.3.4.1 Unit Cell Geometries

CDI modules are available in a variety of shapes and can be utilized as single cells or as stack units composed of numerous cells (Anderson et al., 2010). Generally, symmetrical electrode systems with similar anode and cathode mass ratios are utilized in CDI setups; however, numerous investigations have used asymmetric electrode geometries with varying anode and cathode mass ratios to separate ions from water (Porada et al., 2013).

In the most experiments on CDI procedure, the electrodes are positioned parallel to each other as flow by mode (Figure 2.4 (a)). A stream of water is then sent through the space between the electrodes, which flows via the area where the electrodes are thickest (Porada et al., 2013). Flow-through mode is an alternative to standard CDI geometry (Figure 2.4 (b)). In this geometry, ions are able to immediately get to the electrodes without having to diffuse from the spacer channel (Suss et al., 2012). Another strategy is known as electrostatic ion pumping

(Figure 2.4 (c) (Bourcier et al., 2013). Alternatively, moveable carbon rod electrode wires can be used (Figure 2.4 (d)). Following the electrosorption process, the wires are placed into regeneration water stream for electrode regeneration in which ions are released (Porada et al., 2012).

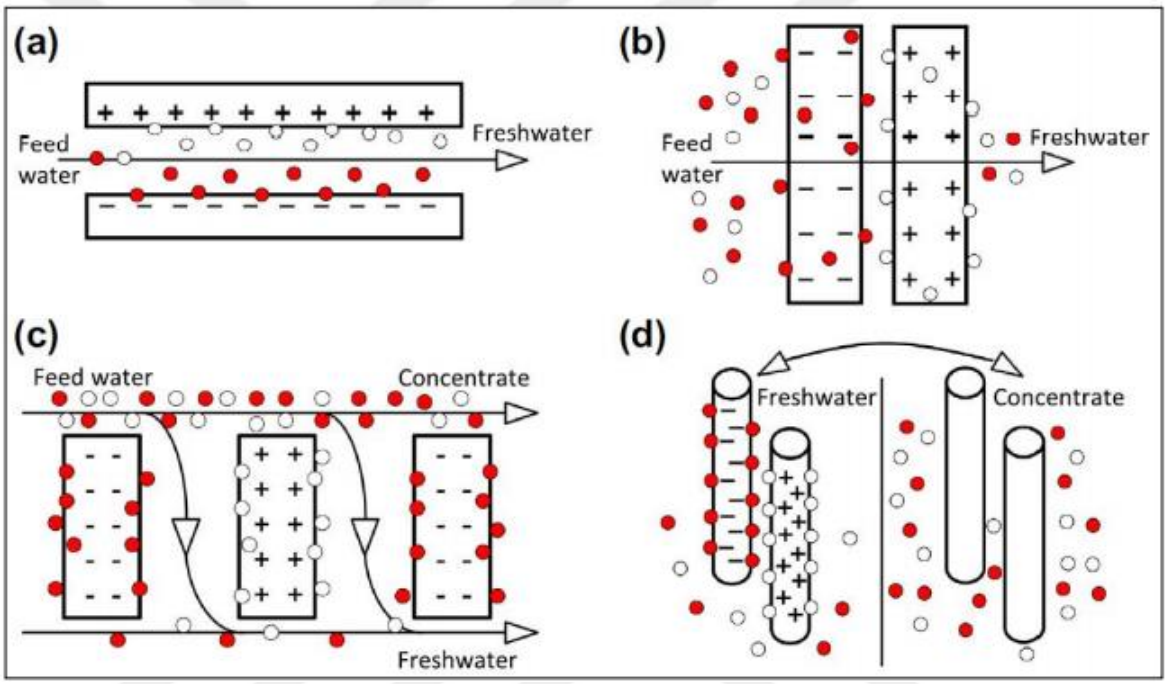


Figure 2.4 CDI system Configurations (Porada et al., 2013)

2.3.4.2 CDI Operation Modes

Although the electrode materials and geometries play a considerable role in the system performance, the operating conditions of the CDI process are significant as well. The two most popular modes of operation are batch and single-pass. With single-pass mode, saline water is pumped continuously to the CDI cell. The extraction process produces a volume of effluent that is collected in another tank. Before the inlet and after outlet of the CDI unit, salinity measurements are taken continuously. These systems may encounter a number of issues, notably variations in the solution's ion concentration over time. Due to both physicochemical qualities (pH, viscosity, conductivity, density), and ion concentration, the water properties (conductivity, viscosity, density) also change. It may be difficult to find stable operating parameters because the changes may necessitate continuous modifications in voltage, current, and water flow to maintain consistent ion removal (Porada et al., 2013; Anderson et al, 2010).

By contrast, batch mode operation systems are the most commonly researched and published configuration of CDI experiments. In batch mode, fixed volume of fed and effluent stream is pumped from and to the same tank. Throughout the experiments, recyclation process of water is repeated in the CDI unit until the salt concentration in water reaches a consistent value. Salinity measurements are taken using inline probes or in the tank (Porada et al., 2013).

2.3.5 CDI Process Operation Parameters

2.3.5.1 Applied Voltage

In CDI, applied voltage is a key operating parameter. It is responsible for the greatest driving force in the ion adsorption process, as well as affecting the electrosorption rate and electrosorption capacity. According to the EDL theory, increasing the voltage applied increases the electrosorption capacity by increasing the electrostatic forces and charge at the electrode/solution interface and decreasing the system resistance. Electrolysis of water and reduction in electrosorption effectiveness of a CDI cell may occur if the electrical potential is increased above a particular limit (Chen et al., 2011).

Numerous experiments have been conducted to determine the impact of applied potential on the ion removal efficiency of the CDI process. Generally, past research has indicated that a positively related to each other, as anticipated. As the system approaches the optimum operation voltage, ion adsorption capacity increases exponentially until a point, at which it begins to decrease due to the increased parasitic effects of the water electrolysis (Oladunni et al., 2018; Liu et al., 2015).

2.3.5.2 Flow rate

Ion adsorption capacity is directly proportional to the flow rate of water in a CDI system. Flow rate is highly important in single-pass experiments with electrode systems, where time duration for salt interaction with the electrodes is proportional to the flow rate. In addition, ion removal efficiency is expected to be high at slower flow rates because the ions in the feed solution are able to stay in contact with the electrodes for a longer time (Mossad & Zou, 2012). Conversely, since all of the water is in touch with the electrodes in batch mode, flow rate has a lesser impact (Chung, 2018).

Previous batch mode experimental tests have indicated that the CDI unit ion adsorption capacity begins to increase up to particular flow rate and then decreases. This is usually the result of flow rates that are too low, leading to insufficient electrosorption; and flow rates that are too high, on the other hand, will increase the pumping force above the electrosorption force, which will reduce the electrosorption capacity of the electrodes. To maintain balance between the driving and electrostatic forces, the flow rate of a CDI system should be set to its optimum value (Chung, 2018).

2.3.5.3 Initial Salt Concentration

Another key component impacting CDI process performance is the initial salt concentration. Understanding the electrosorption behavior of a CDI system is critical when considering various features of the removed ions. As CDI processes are often used for brackish water treatment, investigations focused on salt concentrations under 3,000 ppm as feed water. According to EDL theory, increasing the salt concentration in influent water enhances the ion adsorption capability of a CDI system (Chung, 2018).

Selective ion removal must also be taken into consideration because the type of ionic species is also significant. The major parameters influencing ion electrosorption behavior are the hydrated radius and valence number of the ions. Overall, the majority of related investigations have looked at monovalent (Na^{+}) and divalent (Ca^{+2}, Mg^{+2}) ions. The more the valence of an ion, the greater the electrostatic interaction, and so it is expected that it will have a higher electrosorption ratio (Xu et al., 2008).

In Table 2.3 the salt adsorption capacity of previous research with their operation parameters like (potential difference, flow rate, and NaCl concentration) and materials are summarized.

Table 2.3 Electrosorption capacities obtained with different operation parameters

Electrode Material	NaCl Conc. mg/L	Potential (V)	Flow Rate (ml/min)	Capacity (mg/g)	Reference
AC	50	1.2	7.2	2.6	Hou et al., (2012)
	25	1.2	14	0.25	Zou et al., (2008)
CNT	23	2	25	0.75	Li et al., (2011)
	60	1.2	6	1.3	Wang et al., (2010)
CA	50	1.7	400	1.3	Jung et al., (2007)

2.4 Computational Fluid Dynamics (CFD)

Computational Fluid Dynamics (CFD) is a mathematical method used in the analysis of fluid systems and related phenomena. It is a blend of calculus, physics, and computational science with the goal of describing the flow field. The CFD solver is based on solving the equations of momentum balance and continuity and can also incorporate other physical and chemical processes such as mass and heat transfer and chemical reactions (in heterogeneous or homogeneous systems). CFD has become an essential tool for engineers, particularly in the design and optimization of processes and equipment, due to its advantages such as reducing project costs and time by allowing for simulations and analysis of multiple designs before physical prototypes are manufactured. (Santana et al., 2020).

CFD simulations can be separated into three fundamental stages: 1) Pre-processing (determining the area of interest, creating a numerical mesh, defining initial and boundary conditions, setting mathematical modeling and numerical schemes); 2) Simulation solving (obtaining numerical solutions for the transport equation system); 3) Post-processing (evaluating and analyzing the results) (Santana et al., 2020).

There are many CFD software used in the market like, Ansys, Autodesk, COMSOL, SimScale and others.

2.4.1 ANSYS Software

ANSYS is a powerful engineering simulation software used to simulate and analyze various physical phenomena such as structural, thermal, fluid, electromagnetic, and acoustic behavior. With ANSYS, designers and engineers can virtually test and optimize their designs, reducing the need for physical prototypes and testing, which can save time and cost. The program utilizes finite element analysis to discretize and solve complex mathematical equations that govern the physical behavior of a given system or product (Ansys, 2020; Lecheler, 2022).

One of the most important features of ANSYS is its simulation capabilities for fluid dynamics analysis, which is where ANSYS Fluent comes in. ANSYS Fluent is a computational fluid dynamics (CFD) software that simulates fluid flow, heat transfer, and other related phenomena in various industries such as aerospace, automotive, energy, and chemical engineering (Lecheler, 2022).

ANSYS Fluent is known for its advanced numerical techniques and algorithms that solve complex fluid dynamics problems. Some of these techniques include turbulence modeling, heat transfer, multiphase flows, and combustion modeling. ANSYS Fluent provides a wide range of pre-processing tools that assist in setting up simulations, such as geometry modeling, meshing, and boundary conditions. Additionally, ANSYS Fluent includes a comprehensive library of physical models and material properties to simulate a wide range of real-world fluid problems (Lecheler, 2022).

The software also includes a user-friendly graphical interface that allows users to visualize simulation results and analyze data in real-time. This interface enables users to quickly and efficiently iterate on their designs and improve their products' performance and reliability. By simulating and analyzing fluid dynamics virtually, ANSYS Fluent enables users to improve their product designs, increase efficiency, and reduce costs (Ansys, 2020).

3
EXPERIMENTAL

3.1 Materials

Commercial activated carbon (CPGLF) was supplied from Cargill Company. Polyvinylidene Fluoride (PVDF), N-Methyl-2-pyrrolidone (NMP) and Sodium chloride (NaCl) was purchased from Sigma Aldrich. No further purification was applied to the chemical reagents.

The activated carbon used in electrode preparation is (Calgon CPGLF) a commercial bituminous coal based granular activated carbon. It has a surface are of 648.5 m^2/g, a mean pore radius of 4450 Å and, pore volume of 0.1767 cc/g (Beker et al., 2010).

3.2 Capacitive Electrode Preparation and Characterization

The activated carbon (CPGLF) powder was mixed with PVDF (as binder) with the weight ratio of 10:1. NMP was used as solvent. Obtained slurry was mixed for 30 min, and then left in ultrasonic bath for 30 min. After that, the mixture was casted over a 20*80mm of 30mm*80 mm graphite sheet, which was separated with parafilm. Partly coated graphite sheets were left to dry in the oven at 80°C over night. Uncoated part of the graphite sheet was used to connect the screws carrying the current with the current collector during the desalination experiment.

Cyclic voltammetry (CV) analysis was carried out to characterize the prepared electrodes. In its most basic form, a CV measurement involves selecting a voltage window, scanning the electrode potential while recording the current, and then repeating this process. It provides information about the electrochemical reaction kinetics of the electrode pairs and makes it possible to determine the working voltage window of the produced cell (Frackowiak & Béguin, 2001). Three electrode system were used. Prepared electrode as working electrode, platinum mesh as counter electrode, and Ag/AgCl as reference electrode in 2mM NaCl

solution with the scan rate of 1mV/s and voltage ranges of 0-1.3V. PStrace software was used coupled with potentiostat (PalmSens2, PalmSens CEI) to perform the analysis. The following equation (Eq. 3.1) was used to compute the specific capacitance (C_{CV}) of electrodes (Hou et al.,2012):

$$C_{CV} = \frac{\int_{V_a}^{V_c} I \cdot dV}{m \cdot \vartheta \cdot (V_c - V_a)} \tag{3.1}$$

where, I represents the instant current, ϑ is the scan rate of potential, m is the electrode material mass. V_c is the high potential limit and $V_a$is the low potential limit of voltametric curve.

3.3 Flow Optimization in CDI Cell via CFD

A unique CDI cell with a flow inlet parallel to the flow direction, with an opening at the entry point to obtain homogenous flow distribution and relatively high fluid flow, was designed first by Dr. Dilek Duranoğlu. In this design, there is no need to use external separator, the design provides the needed space between the electrodes by the geometric nature of it. This unique first CDI cell was 3D drawn by using Autodesk Inventor Professional 2022 (academic edition) software package. In this work, this unique CDI design was developed and optimized with the CFD simulation to obtain optimum flow profile. During the simulation process, it was aimed to decrease the dead zone of the flow and to obtain fully homogeneous flow over the electrode. In order to do that some changes were applied to the edges of the cell and corners of the inlet and expansion parts by keeping the electrode holder area constant as 80mm x 20mm over the design study. The impact of cell design on flow regime of CDI cell was investigated using a computational fluid dynamics (CFD) simulation using (ANSYS 2021 R2, academic edition).

Fluid Flow (fluent) analysis solver was used to perform the simulation. It is based on the solution of conservation equations of the transported properties, using an Element-Based Finite Volume Method in the numerical procedure. This CFD package was preferred due to the satisfactory performance on modeling

multicomponent flows in microscale as seen in previous studies. In addition to features such as user-friendly interface, easiness on implementing new materials and source terms, good convergence and numerical stability of such simulations were also taken into account.

In this research, the conservation of total mass (continuity) (Eq. 3.2), momentum (Navier-Stokes) (Eq. 3.3) equations were solved for incompressible, steady-state and laminar flow conditions.

$$\nabla \cdot \mathrm{U} = 0 \tag{3.2}$$

$$\rho\,(U \cdot \nabla U) = -\nabla P + \mu \nabla^2 U + \rho \cdot g \tag{3.3}$$

Where, ρ is the density of the fluid, μ is the dynamic viscosity, U is the Velocity vector, P is the pressure, g is the gravity (He et al., 2021).

The mesh was done by sizing the inlet edges to element division with inflation layers. For calculation, mesh skewness was checked to ensure that it was less than 0.9. In Fluent solver, pressure-based with absolute velocity formulation type was utilized. The gravity effect was in the Z-direction. K-epsilon was selected as viscous model. The boundary condition at the inlet was selected as fluid velocity and atmospheric pressure was set for the outlet. As we deal with the electrode surface, the wall was chosen to be rough and stationary. The residuals for error tolerance were set to be 0.00001 for velocity and continuity and 0.001 for K and epsilon.

After developing three more designs by considering CFD flow simulation results, finally, the optimum CDI cell design were developed. The optimum designed CDI cell was printed with a 3D printer using PLA material via fused deposition modeling FDM technique.

3.4 CDI Setup and Desalination studies

Capacitive desalination performance of optimized CDI cell was measured in recycling batch-mode system demonstrated in Figure 3.1. Before the experiment, distilled water was circulated within the CDI process for 20 min. Then, 2mM NaCl solution was circulated throughout the system for extra 15 min without application of potential, in order to observe the adsorption effect.

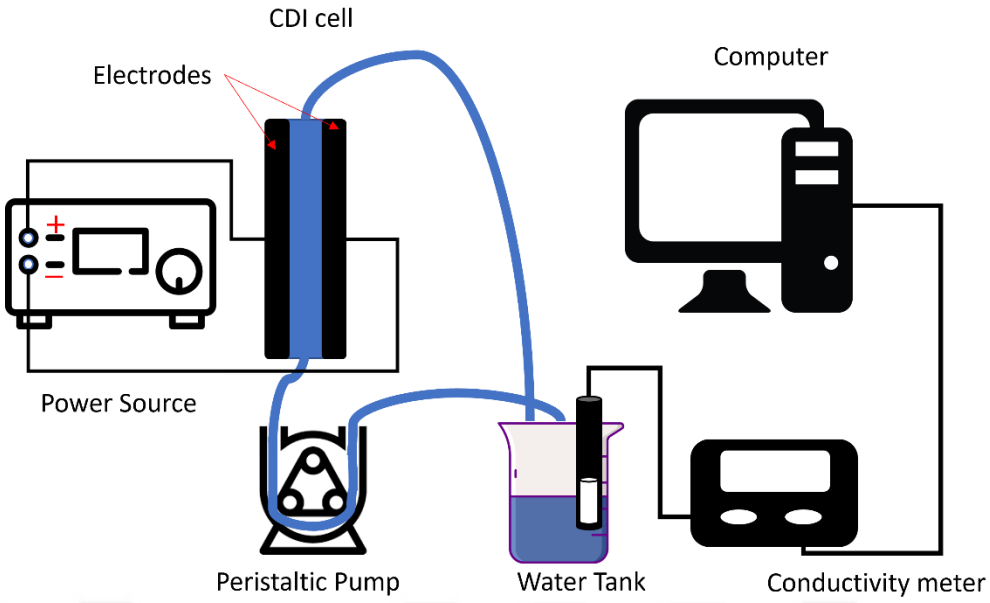


Figure 3.1 CDI experiment setup

In order to investigate the effect of flow rate, 2mM NaCl solution was circulated continuously through the system at two different flow rates (20 and 30 mL/min). Three different voltages (0.9, 1.2, and 1.5V) were applied during the electrosorption while potential difference was set to 0V during all desorption experiments. Three periods (5, 10, 15, 20 min) were investigated for adsorption and desorption during adsorption/ desorption cycles. The electrosorption capacity of the carbon electrodes was calculated based on the change of the bulk solution concentration before and after the application of an electrical voltage in the CDI cell. The salt concentration was followed by measuring the conductivity of the salt solution in the tank. Linear relationship between conductivity and NaCl concentration was already determined before the CDI experiments d . The salt adsorption capacity (SAC) capacity was calculated using the following equation.

$$SAC\left(\frac{mg_{salt}}{g_{carbon}}\right) = \frac{(C_i - C_f)\cdot V_{sol}}{m_{carbon}} \cdot MW_{salt} \qquad (3.4)$$

where, C_i, C_f are the initial and final concentration of the solution (mol/L), respectively. V_{sol} is the volume of the solution circulated in the cell (L). MW_{salt} (g/mol) is the molecular weight of NaCl. m_{carbon} is the mass of carbon film (g).

4
RESULTS AND DISCUSSION

4.1 Properties of Prepared Electrodes

Micro photos of prepared electrodes are shown in (Figure 4.1). As can be seen that the activated carbon was homogeneously casted over the electrodes. The electrode has a graphite mass of 2.54 g with 0.18 g of activated carbon and a 0.61 mm of graphite covered with a 0.16 mm of carbon. The newly prepared electrodes are shown in Figure 4.1a and b while Figure 4.1 c and d shows the electrodes used many times (about 250 cycles). The used carbon displayed a lighter black color due to the continuously exposure to NaCl solution during desalination studies.

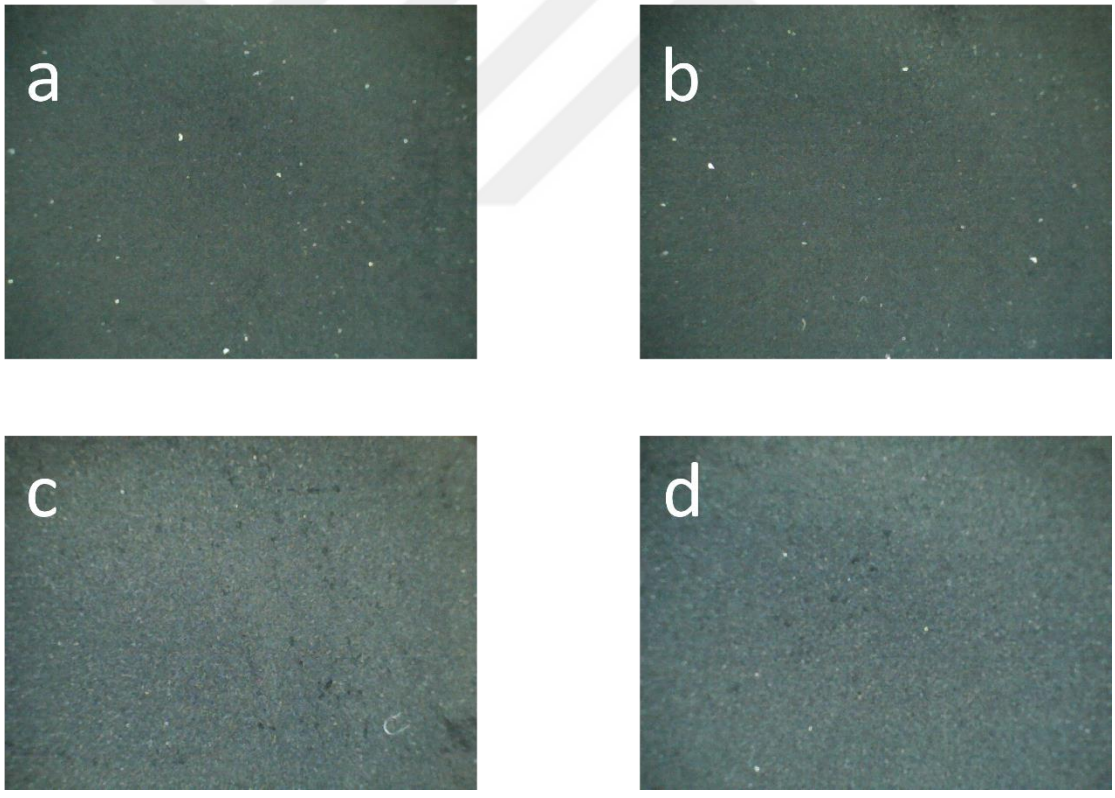


Figure 4.1 Micro photos of prepared electrodes (a, b) fresh prepared electrode, (c, d) spent electrodes

4.2 Cyclic Voltammetry Results

CV curve of prepared electrode can be seen in Figure 4.2. The electrode exhibited a symmetry form demonstrating that Electrical Double Layer (EDL) capacitance of prepared electrodes, and no redox peak was detected. Specific capacitance of the electrode was calculated using Eq (3.1) and found as 8.58 F/g.

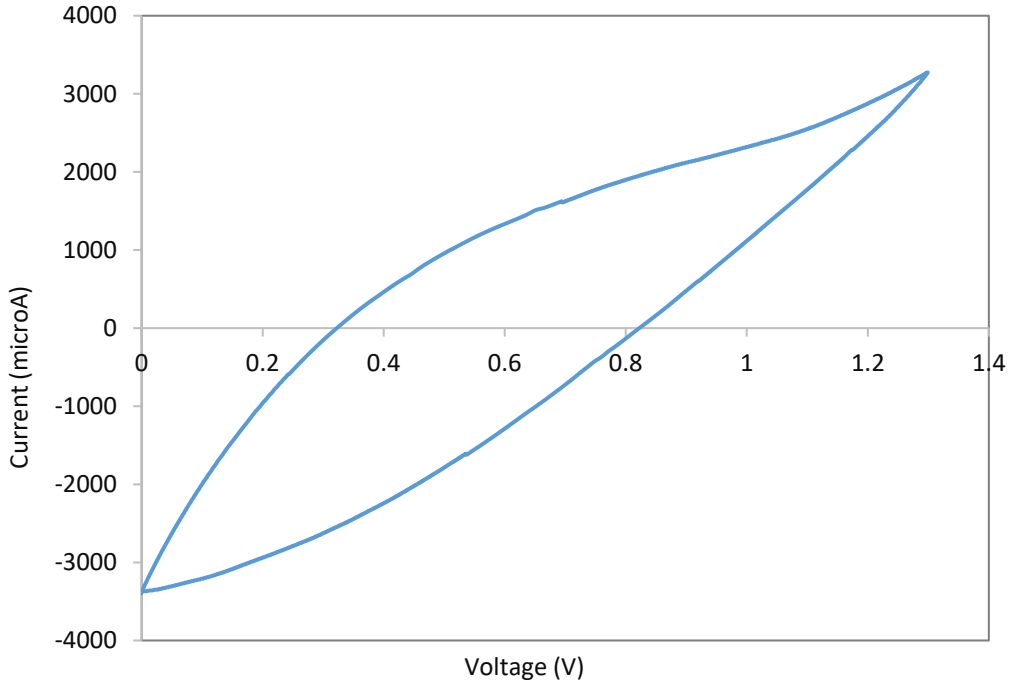


Figure 4.2 Cyclic voltammetry curve of electrode obtained at 1mV/s in 2mM NaCl

4.3 Optimization of Designed CDI Cell Via Flow Simulation

The unique CDI cell has an "inlet" parallel to the flow direction and an "expansion" that provides homogeneous flow distribution. The CDI cell consists of two main identical parts (Figure 4.3). Each part has two layers adjacent to the cell wall. The first layer is the current collector graphite sheet, the second layer is the active capacitive carbon electrode. There is a 1mm gap between two electrodes. Normally in the most CDI cell designs (Hack et al., 2019 and C. Zhang et al., 2019), there is a spacer between electrodes. Creatively in this unique design there

is no need to use a spacer thanks to the design of unique CDI cell. The screws used as current transporter keep the distance between electrodes stable and prevent the electrode movement inside the cell. The screws enter the cell from the opposite part of the cell and stick the electrode to the cell walls.

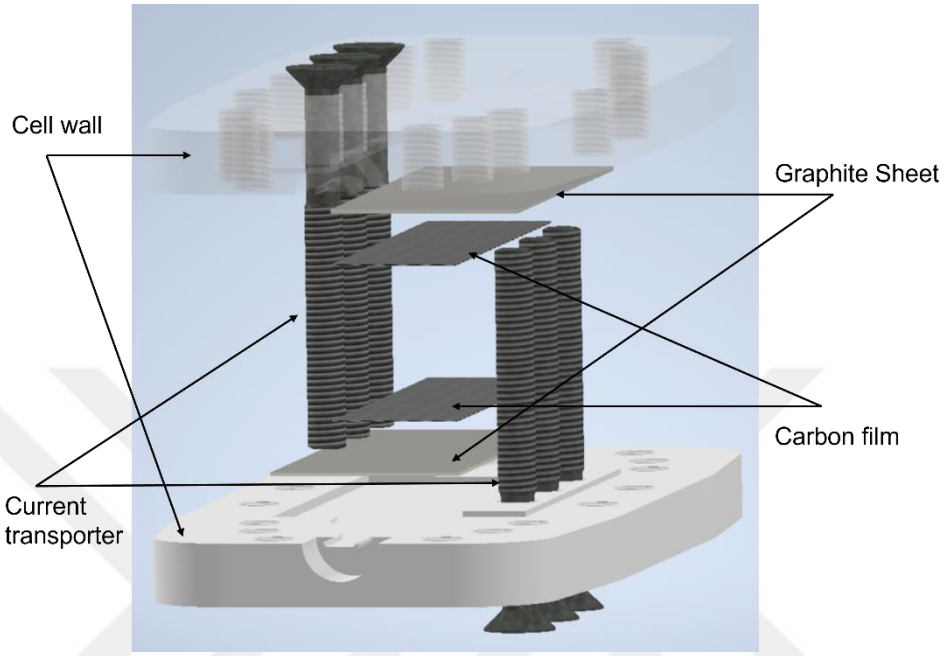


Figure 4.3 Schematic representation of the unique CDI cell

The fluid flow in the CDI cell can be divided into four parts: inlet, expansion, electrode holder and outlet with a length of 20mm, 20mm, and 80mm and 40mm, respectively (Fig. 4.4a). During the optimization of design process, it was aimed to decrease the dead zone of the flow and to obtain fully homogeneous flow over the electrode. The electrode holder area was kept constant as 80mm x 20mm over the design study. The changes were applied to edges of the cell and corners of the inlet and expansion parts. Firstly, the side walls of the cell were curved as shown in Figure 4.4b. Secondly, the corners of the inlet and outlet of the expansion area were also curved (Figure 4.4c). Finally, the expansion part was slightly extended (Figure 4.4d). The optimum cell design shown in Figure 4.4d has a dimension of 12mm for inlet, 38mm for expansion, 80mm for electrode holder and 50mm for outlet part in length. The volume of the flow channel is 2650.7mm^3.

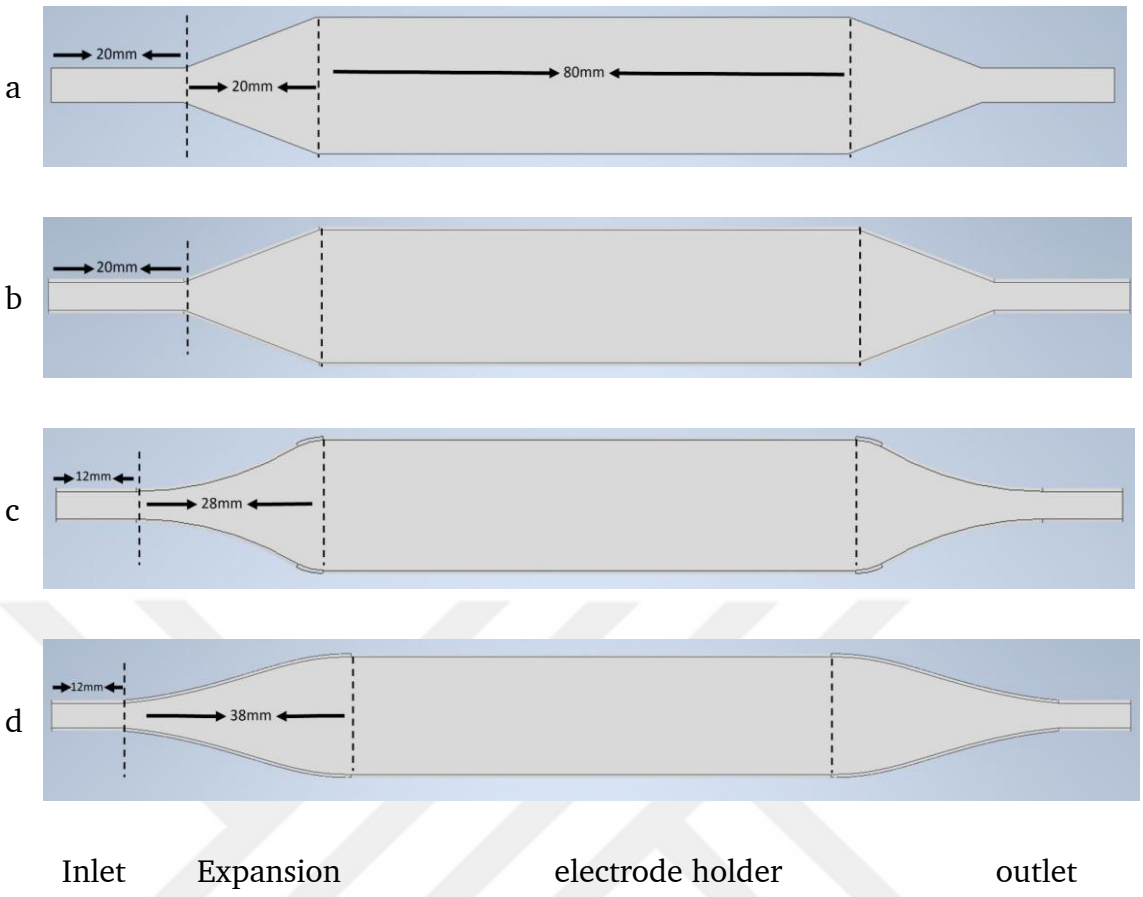


Figure 4.4 Schematic representation of the design steps towards the optimum design. (a) the first design without any modifications, (b) the wall modifications are applied, (c) the corners of expansion part are curved, (d) the expansion part is extended (optimum flow)

4.3.1 Velocity Profile

The velocity profile in the flow channel was investigated for the four types of CDI cells. In general, by changing the cell design towards the optimum design the aim was to minimize the dead zones generated by the walls. Fluid flow velocity profiles obtained via ANSYS software can be seen in Figure 4.5. As shown in Figure 4.5 from a to d, it can be noticed that the dead zone area decreased sharply from the first design towards the optimum one. The velocity profile in the first design (Figure 4.5 a) is not homogeneous compared to the other designs as it has larger dead zone profile and developing flow at the inlet of electrode holder. The second and third design (Figure 4.5 b-c) show almost the same profile from the wall and slightly differ in velocity profile at the inlet of the electrode area. The fourth design

(Figure 4.5 d) shows the smallest dead zone profile with fully developed velocity profile at the inlet of electrode. This decrement in the dead zone profile implies that the effect of rounding the walls and the corners of the flow channel helps in generating a laminar homogeneous flow along the CDI cell. This enhancement will facilitate the maximum usage of electrode area and achieve maximum salt removal capacity. The optimum designed cell was printed with Ender 3 V2 3D printer using PLA material. The optimum CDI cell and its flow simulation result is shown in Figure 4.6.

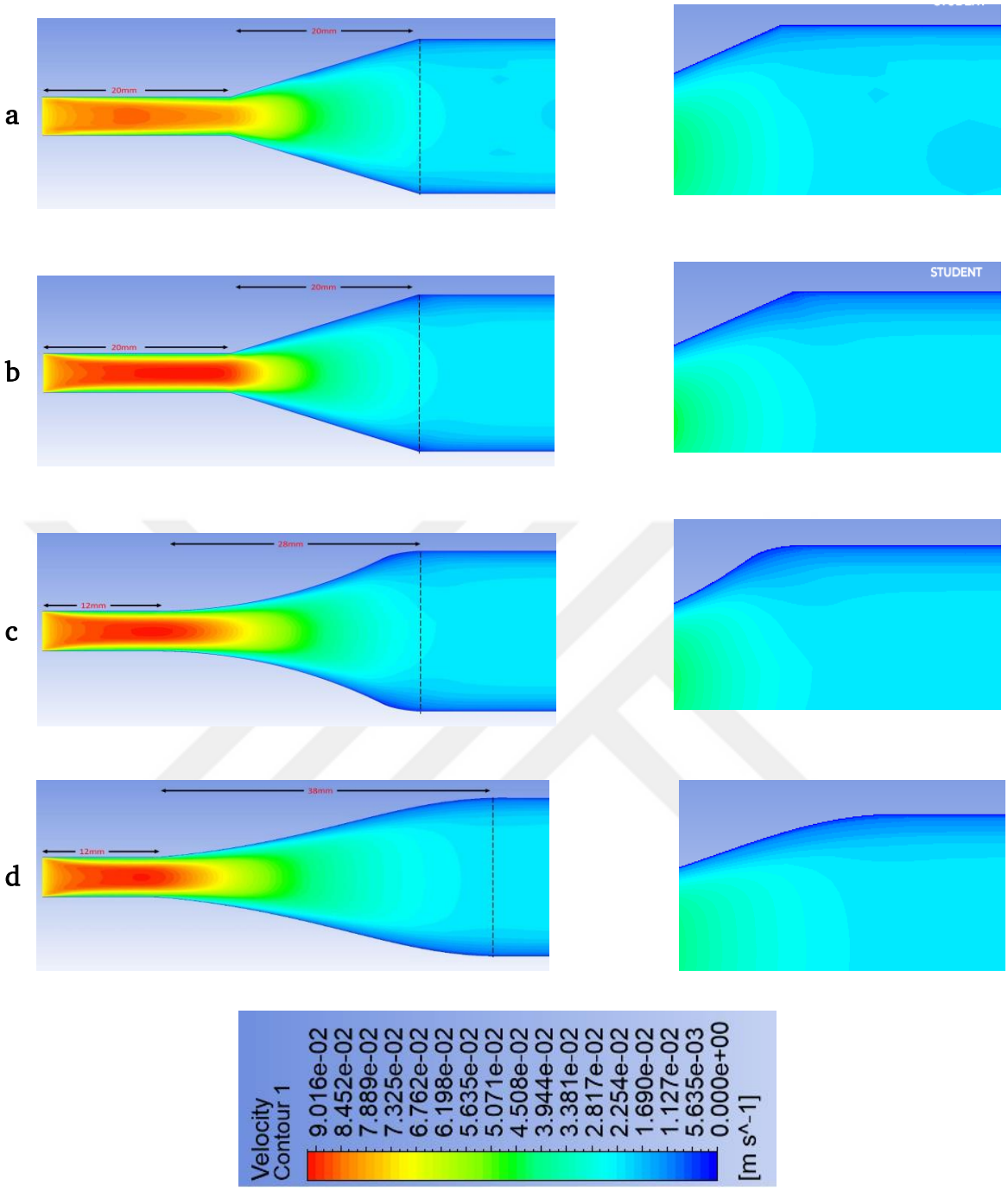


Figure 4.5 Fluid velocity profiles in CDI cell (a) the first design without any modifications, (b) the wall modifications are applied, (c) the corners of expansion part are curved, (d) the expansion part is extended (optimum flow)

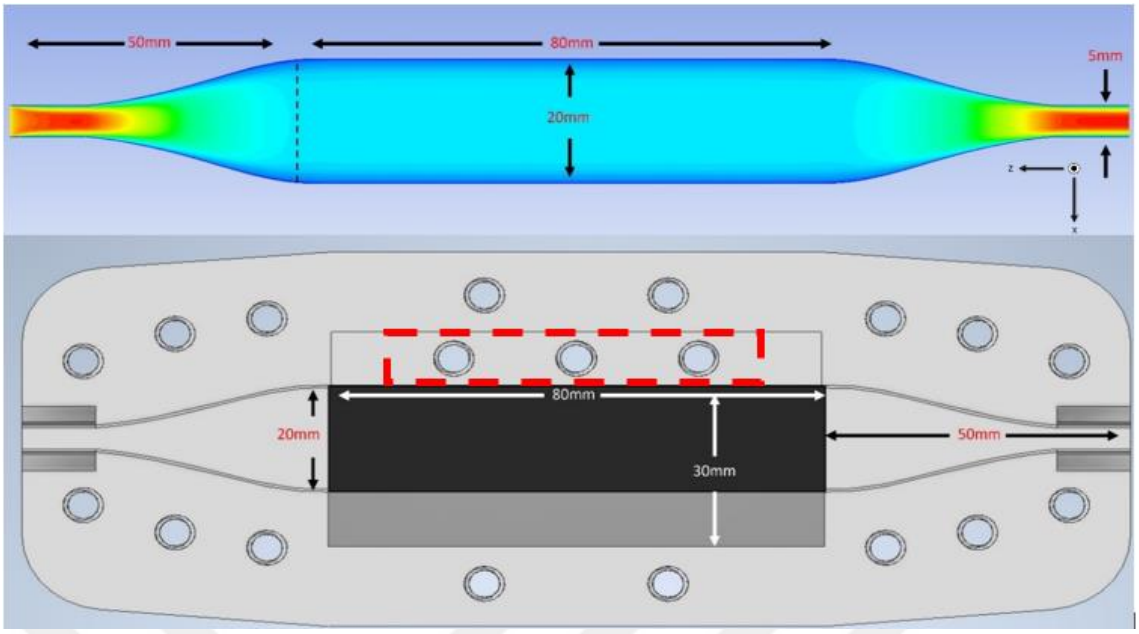


Figure 4.6 Optimum CDI cell design and flow profile

4.3.2 Pressure Drop in CDI cell

The design was also attempts to decrease the pressure drop across the whole cell. The pressure drop obtained from ANSYS simulation for designs shown on Figure 4.5 a, b c and d is 50.7, 49.36, 47.7 and 48.9 Pa, respectively. The pressure drops decreased as we approach the optimum design as a result of wall and corners modifications.

4.3.3 Salt Adsorption Capacity (SAC)

Desalination performance of optimized CDI cell (Figure 4.4d) was tested and compared with the first unique design (Figure 4.4a). The CDI results showed that the performance of the same electrodes were enhanced by 47% in 2mM NaCl (20 mL/min) at 1.2V, and 15 min adsorption period.

4.4 Desalination performance of optimized CDI cell

4.4.1 Effect of Potential Difference

The effect of varying applied potential on salt adsorption capacity (SAC) can be clearly seen in Figure 4.7. Each SAC values were obtained using the average of 8 adsorption/desorption cycles with the 20mL/min flow rate and 2mM NaCl concentration. As can be seen in Figure 4.7, higher SAC values were obtained with

the higher applied potential. This is also confirmed with the results obtained by Jeon et al. 2017). Increasing potential difference causes an increase on the electrostatic force between the solution and electrode surface, hence, leading to a thicker EDL and higher SAC (Liu et al., 2015). In our experiments, the highest SAC of 2.9 mg/g was obtained when applying potential difference of 1.2 V for a 15 min.

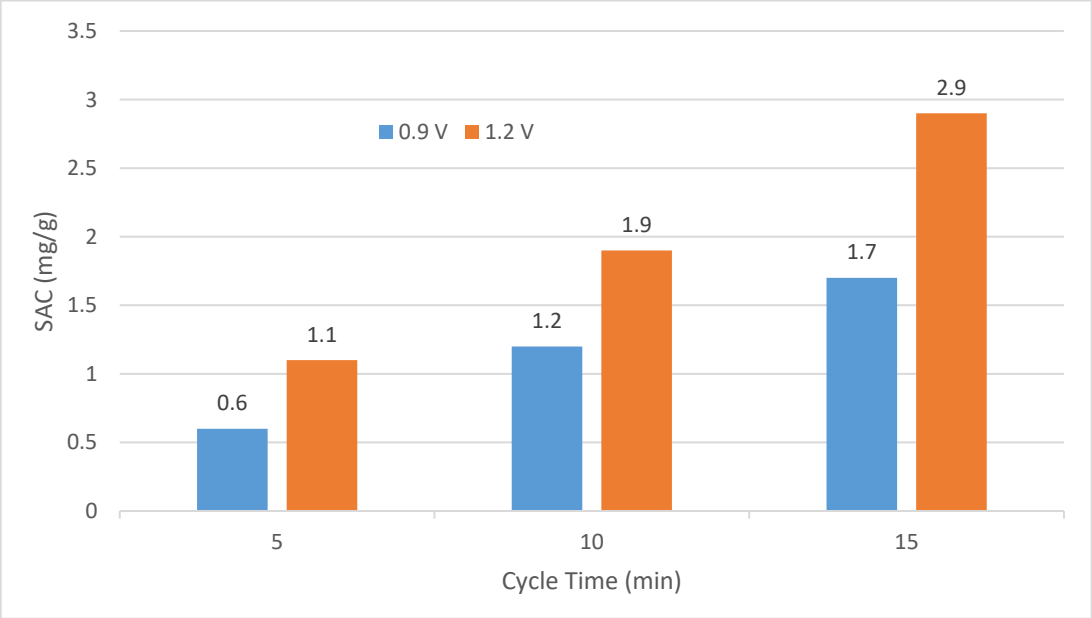


Figure 4.7 Effect of potential difference at different cycle time with the 20mL/min flow rate and 2mM NaCl

4.4.2 Effect of Cycle Time

The effect of cycle time was also investigated in order to optimize the adsorption/desorption period. As can be seen from Figure 4.8 that as the cycle time increased, the SAC of electrode increased until a point where the SAC kept constant. In our study, the system SAC reached its maximum value at 15min and kept constant at longer cycle time (Figure 4.8). This can be explained with the fact that EDL reached its maximum capacity and became saturated at some point. Jeon et al., (2017) have observed that higher SAC was obtained at longer time. Also Liu et al., (2015) reported that any increment in time before saturation point always effect the desalination process positively.

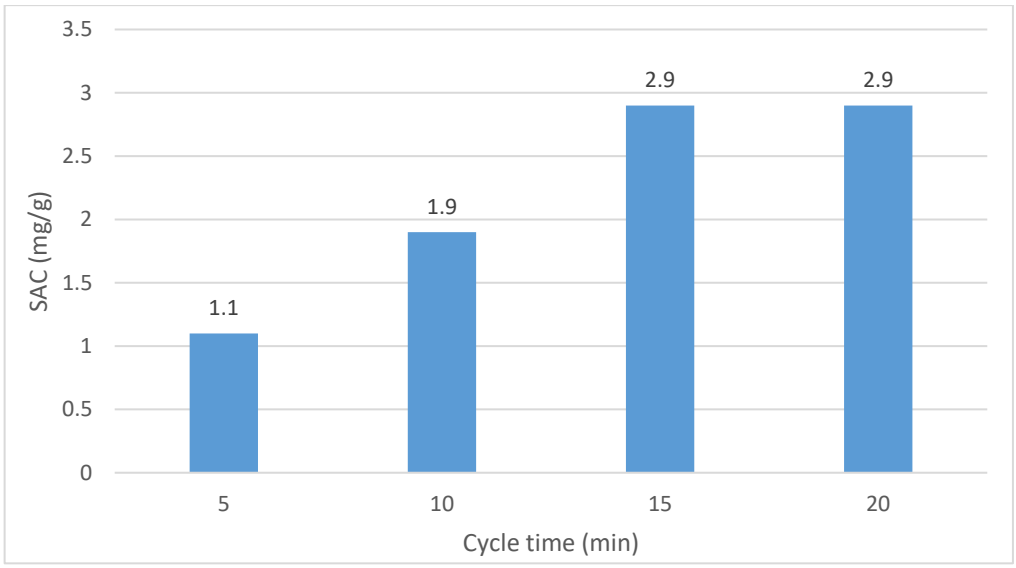


Figure 4.8 Cycle time effect with 20mL/min flow rate and 2mM NaCl at 1.2 V

4.4.3 Effect of Flow Rate

The effect of flow rate on SAC was investigated at fixed potential, salt concentration and time of 1.2 V, 2mM NaCl and at 5, 10 and 15 min, respectively. As it is shown in Figure 4.9, increasing the flow rate slightly decreased SAC because at higher flow rate shorter residence time was experienced in the cell and this led to low adsorption capacity. Jeon et al., (2017) reported that higher adsorption efficiency can be achieved at lower flow rate.

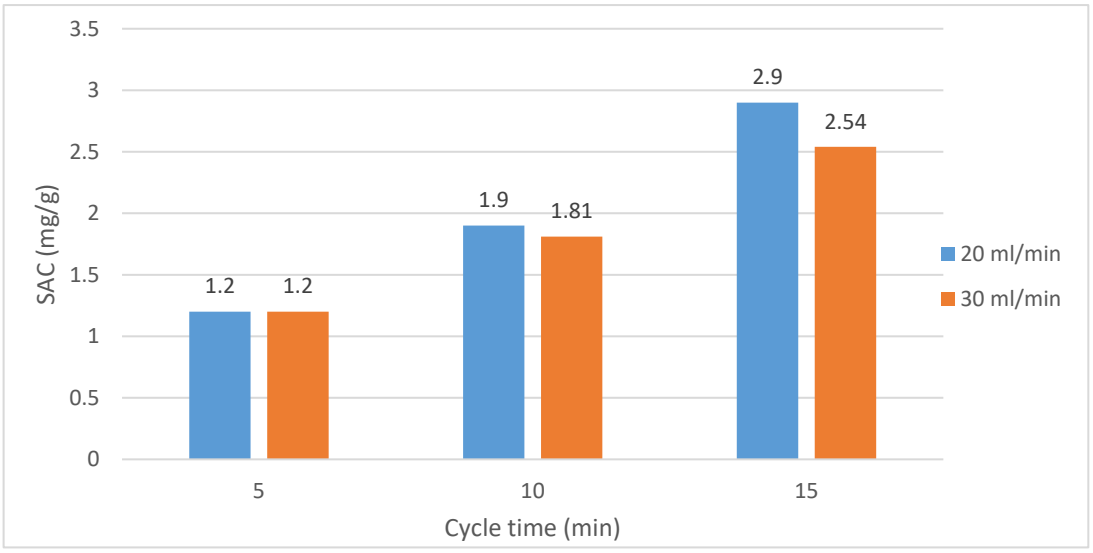


Figure 4.9 Flow rate effect at 1.2V and 15min cycle time

4.4.4 Effect of Salt Concentration

Experiment with different salt concentration was also carried in this work to study the effect of the existence of salt ions in the water on the SAC. The results showed that as the concentration increased the adsorption capacity increased due to the fact that increasing the salt concentration enhance the conductivity of the solution (Chung, 2018). On the other hand, desorption ability of the electrode decreased as shown in Figure 4.10. When lower concentration about 2mM was used, the adsorption and desorption capacity was almost the same. But when higher concentration about 200mM was used, the desorption capacity dropped about 45%. When higher number of ions in the solution are exists, more ions are trapped in the EDL as increasing SAC with the high salt concentration. But when it comes to release to the solution, the EDL tend to hold ions for longer time. This can be explained with the mass transfer resistance due to the higher salt concentration in the solution as it takes more energy to release ions to the solutions. In addition crystallization may occur due to the very high salt concentration on the carbon surface. This effect should be investigated in detail.

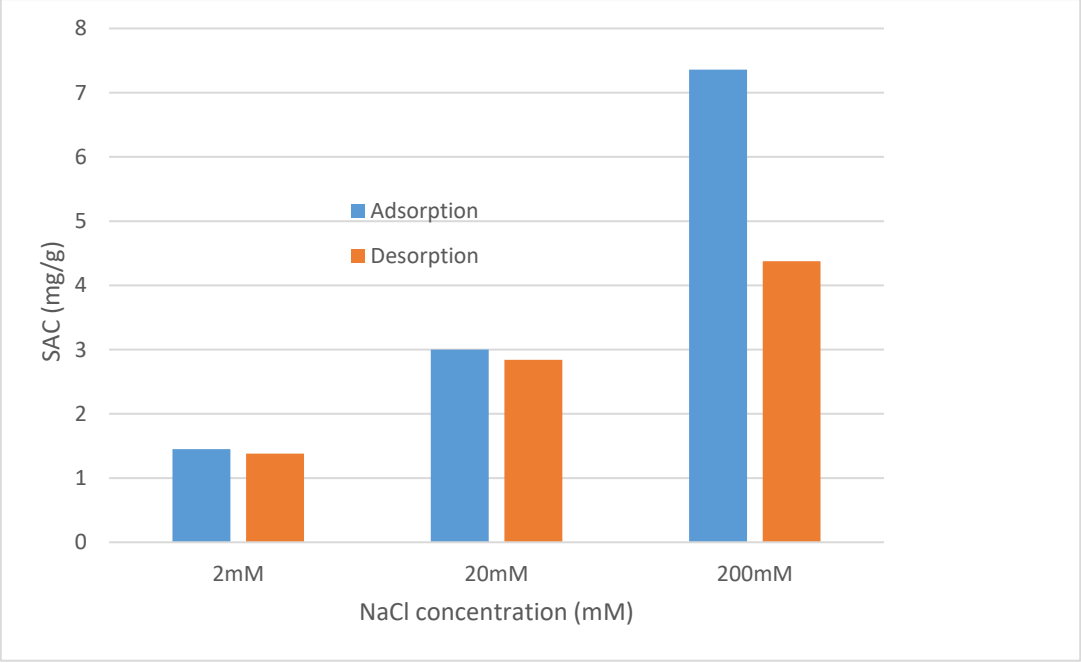


Figure 4.10 Adsorption and desorption capacity at different initial salt concentration

4.4.5 Stability and repeatability

The electrodes exhibited a high stability and longer usability through 220 adsorption/desorption cycles at different flow rates, potential differences, and salt concentrations. As shown in Figure 4.11 the electrodes displayed a stable performance and full regeneration was achieved.

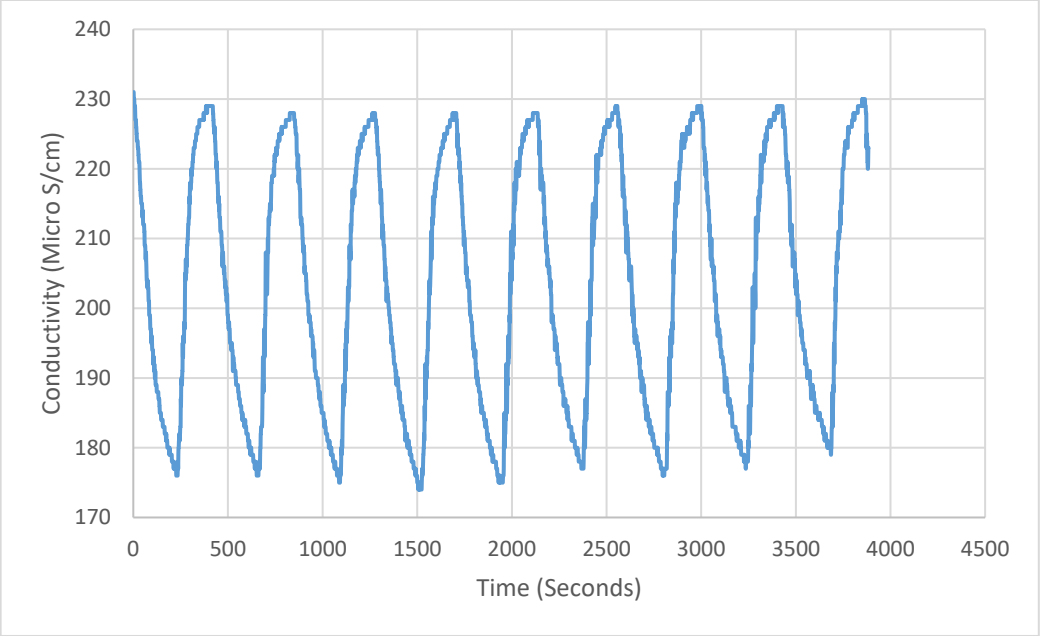


Figure 4.11 Stability and repeatability test (2mM NaCl, 20 mL/min, 1.2 V and,15 min)

The study aimed to develop an optimized CDI cell design that met three key criteria - achieving uniform fluid velocity profile, low pressure drop, and ease of production for scaling up the process. ANSYS flow simulation was used to determine the optimal design parameters for the CDI cell, resulting in a uniform velocity profile and reduced pressure drop. The study also examined the desalination performance of the system, investigating salt adsorption capacity at different applied voltages, flow rates, and adsorption/desorption times. Results demonstrated that the optimized CDI cell design achieved a uniform flow with minimal dead zones, improving salt adsorption efficiency by 47%. The maximum salt adsorption capacity of 2.9 mg/g was achieved at 1.2 V, 20 mL/min flow rate, and 15 min for a full cycle in a 2 mM NaCl solution. As can be seen in Table 5.1, compared to the studies without any additive, an improvement on SAC was obtained with this study. On the other hand, salt adsorption capacity can be

further improved by adding carbon black or graphite powder to electrodes as conductive additives. In conclusion, the study provided valuable insights into optimizing CDI systems and contributed to the development of low-cost, environmentally friendly, and energy-efficient desalination technologies.

Table 5.1 Results obtained from previously published CDI papers

Carbon Type	Additives	Binder	Current Collector	Electrode Dimension	Feed Solution mM NaCl	Capacity (mg/g)	Reference
AC	-	PVDF	-	80 x 80 cm^2	2	2.59	(Hou et al., 2012)
AC	AgPAC MWCNT	polyethylene	Graphite	7.5 cm diameter	10	5.3	(Alencherry et al., 2017)
ACC	-	-	Graphite	25 cm^2	17	8.6	(Laxman et al., 2019)
AC	GO	PVDF	Graphite	6x10 cm^2	7 20.5	5.7	(Folaranmi et al., 2020)
AC	CB	PVDF	Ti	10 cm^2	8.5-34	5.2-8.7	(Lado et al., 2021)
AC	-	PVDF	Graphite	8x3 cm^2	2	2.9	This Work

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