



## Modeling of a continuous water desalination process using directional solvent extraction



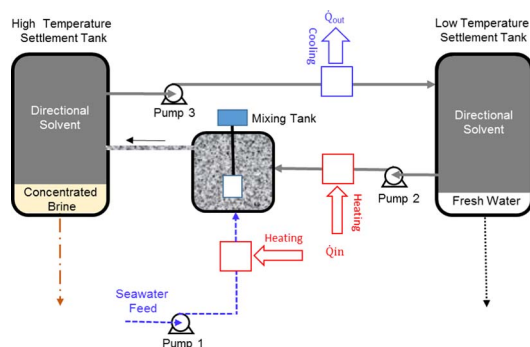
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### GRAPHICAL ABSTRACT



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### ABSTRACT

Directional Solvent Extraction (DSE) is a novel alternative desalination technology to the traditional evaporation and membrane based desalination processes. This new process takes advantage of the fact that water is soluble in some solvents and its solubility increases with temperature. Furthermore, these solvents are insoluble in water and salts do not dissolve in them. These special characteristics of some “directional solvents” have been utilized in this new process to extract fresh water from seawater.

The objective of this paper is to investigate the technical feasibility of a continuous water desalination process using decanoic and octanoic acid as directional solvents. Process modeling was used to predict thermal and electrical energy consumptions for two DSE processes, with and without heat recovery. The effects of highest process temperature, recovery ratio and heat exchanger effectiveness on the thermal energy consumption were studied. The results show that heat recovery significantly reduces the thermal energy consumption. The results also show that octanoic acid has lower thermal and electrical energy consumptions than decanoic acid. Compared to the Multi Stage Flashing (MSF) and Multi Effect Distillation (MED), DSE water desalination process results in higher energy consumption.

In conclusion, the results reveal the need to identify more suitable directional solvents with higher product water yield and lower water solubility in order to facilitate the application of DSE as a potential water desalination process.

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## 1. Introduction

Current desalination technologies can generally be divided into two kinds: (1) evaporation-based processes such as multi-stage flash (MSF) and Multi Effect Distillation (MED); and (2) membrane-based processes like reverse osmosis (RO) [1]. Evaporation-based processes rely on intensive thermal energy to evaporate saline water, and membrane-based processes require the use of high-grade electricity and costly membranes. Relying on desalination as a source of fresh water entails much higher cost compared to withdrawing from conventional fresh water sources. Moreover, these desalination processes either rely on relatively high temperature thermal energy, which is commonly derived from burning fossil fuels, or use electricity. MSF distillation requires thermal energy consumption of about 50 to 80 kWh/m<sup>3</sup> and electrical energy consumption of 2.5 to 5 kWh/m<sup>3</sup> [1–4]. While, MED consumes less thermal energy between 40 and 60 kWh/m<sup>3</sup> and electrical energy consumption around 2.5 kWh/m<sup>3</sup> [3]. RO, on the other hand, requires electrical energy consumption around 3.7 to 8 kWh/m<sup>3</sup> [1,5–10]. The reliance on fossil fuel, which is not renewable, also causes environmental problems such as greenhouse gas emission. Investigating new water desalination processes that are more energy efficient, use renewable energy and/or cost less is a primary goal to achieve sustainable developments.

Due to the potential of utilizing low-grade, low temperature heat sources and membrane-free operation, solvent extraction based desalination was first investigated by Davidson et al. in 1960 [11], where amines were used as directional solvents to extract pure water from saline. Since amine solvents are highly soluble in water, which leads to contamination in the recovered water, this concept did not eventually reach industrial application for water desalination. To overcome the shortcoming of Davidson's study, new extraction solvents, such as soya bean oil, hexanoic acid, octanoic and decanoic acid, were proposed and investigated by Chen and coworkers [12–16]. In these studies, the properties of a directional solvent are described as: 1) water is soluble in solvent; 2) the solubility of water in solvent increases with temperature; 3) the solvent is insoluble in water; and 4) the salt do not dissolve in solvent. Such features will allow extracting fresh water from saline sources while leaving no or little residue, including solvent and salts, in the recovered water. Based on these four properties, a batch process for directional solvent extraction (DSE) has been demonstrated for extracting pure water from saline sources by using solvents like decanoic and octanoic acid. Recently, Bajpayee's study was focused on laboratory experiments to obtain product water yield, recovery water salinity, and recovery ratio for several directional solvents [12]. The study also predicted thermal energy consumption for a continuous process using a simple process modeling. Using octanoic acid, it was found that the energy consumptions for the process without heat recovery was 1250 kWh/m<sup>3</sup>. Assuming 80% heat recovery, the thermal energy consumption was expected to be reduced to 250 kWh/m<sup>3</sup> [12].

A prototype of a continuous DSE process was built where octanoic acid was used as a directional solvent. The system was designed using a centrifuge to separate the octanoic acid from fresh water in order to produce 2.5 gal of water per day [14]. Difficulty in operating the centrifuge in this prototype was reported and recommendation was given to optimize the centrifuge for this process. Luo et al. [15] and Rish et al. [16] investigated solubility properties between directional solvents such as decanoic acid and water by using free energy calculations. At molecular level, inter diffusion processes of decanoic acid and water were modeled using molecular dynamic simulations, which was proposed as an *in-silico* method to simulate and identify new directional solvents.

A follow-up paper by Sanap et al. [17] studied a continuous DSE process using octanoic acid. To predict the liquid-liquid equilibria properties of octanoic acid and seawater, limited experiments were performed for mixtures of water, sodium chloride and octanoic acid at different temperatures. The thermal energy consumption was

calculated to be between 318 and 330 kWh/m<sup>3</sup> and the pump power consumption was estimated to be between 7 and 10 kWh/m<sup>3</sup>.

In summary, most of the research and publications studied a batch DSE process to demonstrate the basic concept of extracting fresh water from salty sea-water using directional solvents [11–15]. Few studies considered a continuous DSE process [12,14,17]. None of these studies considered heat exchanger network synthesis to maximize heat recovery and minimize the heat input. Furthermore, the electrical energy consumption for mixing and separation processes were ignored when estimating the total electrical energy consumption.

The objective of this paper is to investigate the technical feasibility for a continuous water desalination process using decanoic and octanoic acid as directional solvents. Two process configurations were considered and their performance were compared: one was modeled as a simple system with no heat recovery and the other was modeled with maximum heat recovery. The thermal energy consumption was predicted based on product water yield measurements by Bajpayee [12]. The electrical energy consumption, on the other hand, was estimated for pumping, mixing and separating the sea water and the directional solvent. The impacts of highest process temperature, recovery ratio and heat exchanger effectiveness on the thermal and electrical energy consumption were studied.

## 2. Performance indices for continuous DSE process

In the continuous DSE process, the product water yield,  $Y$ , is defined as a mass flow rate of purified water,  $\dot{m}_w$ , per unit mass flow rate of solvent,  $\dot{m}_{so}$ .

$$Y = \dot{m}_w / \dot{m}_{so} \quad (1)$$

The recovery ratio,  $RR$ , is defined as the mass flow rate of purified product water to the mass flow rate of seawater feed,  $\dot{m}_{sw}$  [12].

$$RR = \dot{m}_w / \dot{m}_{sw} \quad (2)$$

The heat exchanger effectiveness,  $\epsilon$ , is defined as the ratio of actual heat transfer,  $\dot{Q}$ , to the maximum heat transfer,  $\dot{Q}_{max}$ .

$$\epsilon = \dot{Q} / \dot{Q}_{max} \quad (3)$$

The thermal energy consumption,  $TEC$ , is defined as the amount of heat input consumed per volume of purified water, in kWh/m<sup>3</sup>.

$$TEC = \dot{Q}_{in} / \dot{V}_w \quad (4)$$

where  $\dot{Q}_{in}$  is the heat input and  $\dot{V}_w$  is the volume flow rate of purified water.

Pumping electrical energy consumption,  $EEC_p$ , is defined as the amount of electrical energy per volume of purified water, in kWh/m<sup>3</sup>.

$$EEC_p = \dot{P}_p / \dot{V}_w \quad (5)$$

Mixing electrical energy consumption,  $EEC_m$  is defined as the amount of mixing power requirement per volume of purified water in kWh/m<sup>3</sup>.

$$EEC_m = \dot{P}_m / \dot{V}_w \quad (6)$$

Separation electrical energy consumption,  $EEC_s$  is defined as the amount of separation power requirement per volume of purified water in kWh/m<sup>3</sup>.

$$EEC_s = \dot{P}_s / \dot{V}_w \quad (7)$$

where  $\dot{P}_p$ ,  $\dot{P}_m$  and  $\dot{P}_s$  are the electrical power requirements by the pumping, mixing and separation processes of DSE, respectively.

Total electrical energy consumption,  $EEC_{total}$  is then given by the following equation:

$$EEC_{total} = EEC_p + EEC_m + EEC_s \quad (8)$$

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