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Simulation and Optimization of Solar Desalination Plant Using Aspen Plus Simulation Software

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Abstract

Of the total global water, 94% is salt water from the oceans and the remaining 6% is fresh. The shortage of fresh water is a problem that has continued to challenge third world countries, and over time has become increasingly evident in developed nations around the globe. With a combination of contributing issues such as overpopulation and changes in weather and climatic conditions, the demand for alternate approaches to fresh potable water supply has increased dramatically. The paper develops a computational model to simulate the performance of a small scale solar desalination plant. The model is validated with experimental results found in the literature. The validated model is used to optimize the functional parameters of a desalination plant and in turn, enhance the recovery rate and product quality of the system. The model is suitable for brackish and seawater desalting applications specific to the climatic conditions of coastal Queensland, Australia. Aspen Plus is the process simulation software that was used for the modelling. The outcomes of the study is a validated process simulation model of a small scale solar desalination plant, optimization of this model for better utilization of current technologies and methods of improving performance, efficiency and recovery and reducing operational limitations.

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Keywords: Solar desalination plant, Aspen Plus software, Simulation, Optimisation.

1. Introduction

Among the water reserves in this world, nearly 6% is fresh water and remaining is saline water. Approximately 27% of all fresh water reserves are in glaciers with 72% located underground with the remaining 1% accounted for in the limited fresh water dams, streams, lakes and river systems throughout the world. Desalting technologies have evolved over the last 50, impacting lives with considerable effect especially in remote regions of the Middle East and

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North Africa where the lack of fresh water was previously impeding development. A major development and realization of the potential of desalination was first discovered in the mid 1940's during WWII when various military camps in arid areas required potable water for the troops. Following the war, further industrial advances continued into the 1960's [1]. Over time, the maturity of both desalination processes and renewable energy sources have been proven by social acceptance from implementations causing growth and development of both technologies [2, 3].

Australia is both the driest inhabited continent on earth and the highest consumer of water per capita by international standards [4]. Of all continents it has the smallest area of permanent wetlands, the least river water and the lowest run off along with the most variable rainfall records in the world [4]. In recent times, a combination of technology advancements and actions taken by leading authorities and governments has seen an increased awareness in the possibilities of alternative fresh water sources. After studies undertaken as a part of the National Water and Resources Audit found there would be a likely decline in the quality of water supplies over the next 50 years [5], measures including the introduction of zoned water restriction regulations in Australia have helped to stem the usage of the diminishing fresh water reserves. Additionally, extensive investigations and research have provided promising alternative methods of obtaining potable water.

Of all the investigated technologies, desalination has emerged as being one of the most promising solutions to providing an alternative means of fresh water supply. Considering its climatic conditions and suitability, until recent times, Australia has comparatively limited operational expertise and experience in desalination technologies and falls behind world leaders in the Middle East and North Africa where almost half of the world's desalting capacity lies. Isolated mining towns and small communities as well as industrial processes such as power stations that require exceedingly high qualities of water are the main users of desalination technologies in Australia [5]. Over the past decade, several plants in Australia have been constructed or have been proposed for public potable water supply such as the Perth based 130ML/day RO plant which has the potential to expand with additional extensions. Desalination technology has also been introduced to offset the amount of potable water used for purposes other than drinking. In an Australian first, a water mining treatment process operating at Rocks Riverside Park in Queensland utilizes a low cost, sustainable natural treatment and filtration process to convert wastewater to quality non potable drinking water for parkland irrigation saving up to 360kL of potable water daily [6].

In 2009, the Commonwealth Scientific and Industrial Research Organization (CSIRO) conducted a report to investigate the status of desalination on a national scale. Of the 46 desalination plants investigated, 45 operated as reverse osmosis (RO) plants. It was found by comparison with Australia's total potable, industrial and agricultural water consumption in 2004-05 (51.5 GL/day), the amount of desalted water used in 2008 is 0.57% of that total (0.294 GL/day) [5]. These figures represent the potential Australia has to develop and implement desalination technology and with further reports showing that the cost of seawater RO plants have fallen by 300% in the past 15 years [7], it is now more economically and financially feasible than ever.

The main aim of this study was to develop a process simulation model of a small scale solar desalination plant using programs and software that decompose the process into its constituent elements for the purpose of predicting performance using analysis techniques. These process characteristics included feed flow rates, temperatures, pressures, compositions, and specific properties of equipment. Through the input parameters and design equations, the model considered and simulated the three stages of the process including feed pre-treatments, structure and desalination technique and the final permeate and retentate outputs. These outputs were then validated against data from recognized past studies which had been completed using geographically appropriate data that coincided with the Central Queensland area, Australia.

Once the outputs were verified, the model was then adjusted and optimized by altering a number of variables including adjustments to the configuration of the desalination process, quality of feed water, level of pre-treatment and extent of filtration in an effort to increase the performance, recovery rate and efficiency, thus impacting on the required input power, magnitude of brine waste, maintenance requirements and running costs. The purpose of the optimization was to determine the most realistically achievable, sustainable and environmentally responsible small scale arrangement to produce potable water for a community subject to a typical Queensland climate with access to abundant supply of brackish or seawater.

2. Methodology and Experimental Measurement

2.1. Component of the System

The system to be replicated and used for validation purposes consists of three main sections throughout the entire desalination process, pre-treatment and pressurization, power supply and the RO membrane arrangement. The system under investigation has no grid connection and is powered completely from solar energy obtained through a photovoltaic arrangement. Figure 1 outlines the system schematic with arrows outlining direction of flow. The system makes use of a salt water feed intake from a beach well before introducing a simple coarse filter pre-treatment ensuring suspended solids are removed before the feed stream is pressurized through the positive displacement pump which is powered by the solar PV array. A flow meter and pressure relief valve monitor the flow rate and pressure of the system downstream of the pump before the membrane arrangement desalts the feed into the two final output streams of brine reject and the product permeate.

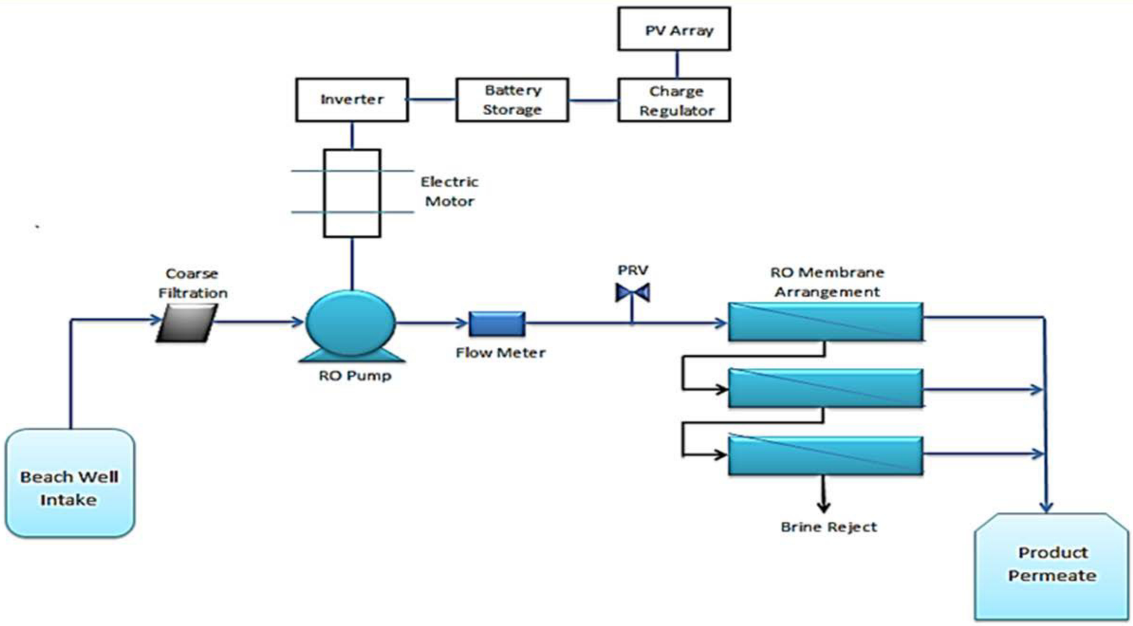

Figure 1: Reference Data System Schematic.

Power Source: Harnessing solar energy are 10 off 80W Sharp NE-80EJEA poly-crystalline panels connected in parallel. This PV array gives a DC output which is delivered to a Xantrex DR1512E 1500W inverter with integrated battery storage and charging element. The inverter transforms the DC supply into an AC voltage before it reaches the AC induction motor. Table 1 summarizes characteristics of the PV modules and the main PV system elements.

Pressure Source: The pump powered by the electric motor is a Hydra-cell D/G-03X positive displacement pump. With the pressure and flow rate of the feed stream being two influential characteristics on the output of the system, these are monitored and mediated by both a flow meter and pressure reducing valve. These elements are critical in the consideration of both the simulation and experimental operation as they ensure large fluctuations are eliminated allowing single values to be inputted into a model while maximum design specifications for both the pump and RO membranes is not exceeded. These elements are also versatile instruments in practical applications to mimic simulation results once optimization has been carried out.

Desalination Source: The membrane configuration used in the referenced data set is a 3 membrane arrangement in series. Each product stream feeds back into one permeate line while the brine stream feed the preceding membrane before discharging from the final membrane. Although additional membranes results in a greater pressure loss over the series configuration, investigations from the reference data suggest a smaller applied pressure is required for an increased recovery rate. The retentate discharge is also at a pressure that an energy recovery device can be implemented into the system to enhance the prospect of turning the configuration into an energy generating operation. In simulating the above system, the AspenPlus software [8] allows the user to define the feed water characteristics. The temperature, pressure, volumetric flow rate and concentration are among the original input variables used to define the feed water.

Table 1: PV Module and System Characteristics

Module Characteristics System Elements		System Elements	
Cell Type	Poly-Crystalline Silicon	PV Array	10 off Sharp NE-80EJEA poly-crystalline panels
Number of Cells	36 (series)	Charge Regulator	Plasmatronics PL60 60A Solar Regulator
Open Circuit Voltage	21.6V		
Maximum Power Voltage	17.3	Battery	4 off US185, 12V, 195A.hr flooded cell lead acid battery in parallel
Short Circuit Current	5.16		
Maximum Power Current	4.63	Inverter	Xantrex DR1512E 1500W
Maximum Power	80W	Electric Motor	Baldor EL3507 115/230V, 559W, 0.75hp AC induction motor

2.2 Input Data

Feed Water Characteristics: With the model being proposed to simulate operation in the climatic conditions of Yeppoon in Central Queensland, feed water characteristics were chosen to replicate those in the case study location. These properties of temperature, pressure (based on osmotic pressure of the feed water concentration) and salinity concentration are outlined in Table 2 as used in the simulation model. The system was designed to produce 0.5m3/day product water under a 6 hour operational cycle coinciding with the time of day that yields the highest solar potential. The feed water flow rates used were defined in three arrangements as the model was developed. The single, double and triple membrane arrangements in series adopted varying flow rates. Because of this, the development of the Aspen Plus model adopted the same progression to ensure validation was accurate. The variable feed flow rates used for validation are shown in Table 3

Table 2: Feed water characteristics used for validation and simulations

Description	Value
Temperature (oC)	25
Pressure (bar)	34.5
Feed concentration (ppm)	35

Table 3: Feed water flow rates used for validation and simulations

System arrangement	Feed flow rate (m3/hr)
Single	0.830
Double	0.506
Triple	0.414

Membrane Characteristics: The modelled and simulated membrane was a spiral wound SWC-2540 manufactured by Hydranautics and used in the simulation. This particular membrane was of a thin film composite polyamide construction and had an active area of 2.37m2. The membrane performance and efficiency is based on the primary characteristics of percentage salt rejection and maximum permeate flow relative to geometry under ideal conditions. As outlined on the manufacturer's website, these properties are 99.4% and 2.0m3/day respectively. Table 4 outlines the maximum application conditions at which the membrane is designed for general use. For specific or prolonged use, operation at more conservative levels would ensure the longevity and performance of the device. Dimensions A, B and C mentioned in the table are described in Figure 2.

Table 4: Maximum application conditions [9]

In put parameter	Values
Maximum Applied Pressure	6.9 MPa
Maximum Chlorine Concentration (not applicable for current model)	< 0.1 ppm
Maximum Operating Temperature	45^{o}C
pH Range (for continuous use)	3.0 – 10.0
Maximum Feed Water Turbidity	1.0 NTU
Maximum Feed Flow	23 L/m
Maximum Pressure Drop for each Element	70 KPa
Dimension A	1016 mm
Dimension B	61 mm
Dimension C	19.1 mm

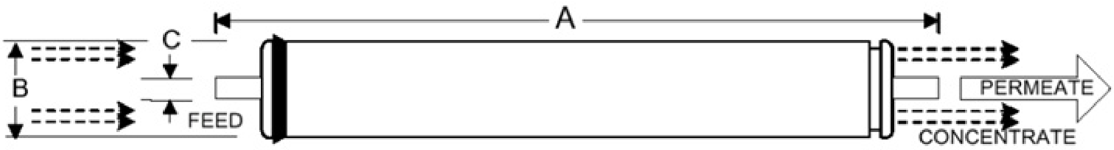

Figure 2: Membrane dimension

Product Characteristics: The primary aspect of the permeate that was required to be accurately simulated to achieve validation was flow rate. As a result of known feed flow, the recovery rate was also an indication of validity of the model. Table 4 shows the properties of the permeate for the corresponding system arrangements.

Table 5: Product Permeate Properties (Schrader, Rasul 2008)

System Property	Single Arrangement	Double Arrangement	Triple Arrangement
Feed Flow (m3/hr)	0.83	0.506	0.414
Permeate Flow (m3/hr)	0.083	0.136	0.166
Recovery (%)	10	16.4	20.05

The data proposed that the product output from the system should be free of any traces of sodium chloride or other minor saline elements. With the ideal salt rejection factor of the membrane being 99.4%, this is not a realistic target nor is it possible with this model of membrane. According to the Western Australian Department of Health, potable water can contain traces of NaCl of up to 180mg/L (180ppm) for taste based on an aesthetic guideline level from the ADWG. It was expected for this simulation, the product water would be suitable for uses equivalent to recycled water and not for consumption. The expected return of permeate concentration for salt water RO processes with a feed water concentration in excess of 32,000mg/L is no greater than 500mg/L. With this the accepted industry norm outlined by Hoang et. al. [5], results of less than 500ppm will be acceptable and deemed accurate.

2.3 Simulation Techniques and Assumptions

Aspen Plus software offers the user a number of existing libraries containing product blocks with defined settings ranging from pumps and centrifuges to filters, splitters and evaporators. The program also allows the options to customize a user defined unit operation block which specifies a process that isn't captured or can be modelled using the items within the existing libraries. To simulate the RO membrane, a process that selectively separates the feed stream into two streams based on the membrane characteristics needed to be selected. With the RO membrane acting as a combination of blocks such as filters and splitters, the option of using defined blocks was deemed inaccurate and unsuitable, meaning a customized unit operation block was needed to model the membrane. Using the user block option in the Aspen Plus library, the Hydranautics SWC-2540 membrane was created and simulated in single, double and triple series arrangements before being validated and sequentially optimized. Throughout the development, simulation and validation of the Aspen Plus model, there were a number of assumptions that were made which are listed below.

- The effect of scale build up, system purity and prime running conditions have negligible effects on the design and effectiveness of the membrane.
- The properties of the feed water remain constant during the treatment meaning, the TDS level does not alter along with temperature, level of suspended solids and additional pre-treatment requirements due to unforeseen contaminants or a change in outside conditions.
- Due to the model being validated against the existing theoretical result, an assumption was made that appropriate measures were taken during the study to ensure that the results collected are accurate and correct. In the event that the results were considered unrealistic such as the saline concentration in the product streams, realistic limits and boundaries were set to ensure accurate validation.
- Material degradation during the life of the simulated system was negligible and did not affect the outcome of the simulations.
- Membrane elements and specifications were all taken at a maximum during input calculations and when determining performance characteristics of the model.

3. Modelling and Simulation Results and Discussion

In order to develop a validated model against the design data, the Aspen Plus model adopted the single to triple membrane series arrangement progression. The model was tested as each membrane was added to the system to ensure validation of the simulation was achieved. Figure 3 outline the model as it is developed from a single membrane to the triple membrane series arrangement validated and used in the optimizations process. For means of validation, the primary results returned from the simulations were those comparable to the validation data including permeate flow rate and system recovery percentage. Although the product concentration of the validation data was neglected, this aspect of the permeate was monitored throughout the simulations to ensure it remained below 500ppm as expected according to Hoang et. al. [5]. Other properties of the system were also checked throughout modelling for any adverse or unexpected results that could have inhibited validation of the simulation. The final simulations for each arrangement were all completed 'normally' and without errors.

3.1 Model Validation

The validation process was carried out progressively as the model was developed from a single membrane system to the three membrane series arrangement to ensure the model obtained and maintained accuracy until the final model was established. The flow rate which corresponds directly to the system recovery along with the boundary limits of permeate concentration were the properties used to determine and establish a validated model. In order to determine the validity of each model progression, the percentage difference was found for these characteristics with the maximum allowable variation set to 2%. Table 6 shows a summary of the simulated result, the validation data and the variation between the two sets of data.

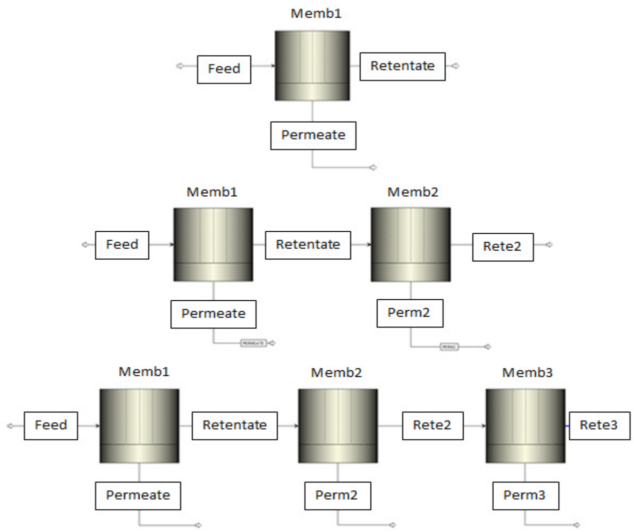

Figure 3: Membrane series model development schematic

The small inaccuracies that were recorded can be assumed to have originated from the differences in the allowable concentrate levels in the simulated and validation permeates. With a maximum of 466ppm difference in this level, the membrane flow characteristics that were calculated in the validation data would have been modelled to an unrealistic level, generating performance characteristics such as salt rejection coefficients beyond the capacity of the SWC-2540 membrane. Although errors were apparent in the simulations, the developed model coincides with the validation data within the accepted error limits of 2% and less than 500ppm TDS concentration. With this the case, the model is deemed as valid and optimization investigations can be carried out.

Table 6: Validation Data and Variation Percentages

Arrangement	Simulation Permeate Flow Rate (L/hr)	Validation Permeate Flow Rate (L/hr)	Difference (%)	Maximum Permeate Concentration (ppm)
Single	83.16	83	0.19	292
Double	136.09	136	0.07	399
Triple	166.01	166	0.01	466

2.2 Model Optimization

The optimization process adopted a structured form which altered each feed characteristic of the triple membrane arrangement one at a time within suitable limits. Results were recorded after each simulation which focused predominantly on the flow rate and concentration of the permeate stream and the concentration and pressure of the brine waste. The optimum settings for each parameter are recognized and discussed with regard to possible implementation and the effectiveness of altering the system. For comparison and discussion purposes, the recorded data was graphed and is shown in the preceding discussion.

Temperature: The feed input values used for the temperature optimization simulations were as per the triple arrangement validation simulation with the exception of the variable temperature property. The temperature ranged between 10 oC and 40 oC at increments of 1 oC and small linear improvements were seen as temperature dropped below the initial simulation temperature of 25 °C. No changes were seen in product concentration or pressure drop across the membrane modules. Figure 4 gives an indication of the total product flow from the system as a variable feed temperature is introduced. As can be seen from the plot, the system returns small increases as the temperature decreases. Figure 5 gives a graphical display of the percentage improvements due to the alteration of the feed water temperature. As shown, the maximum increase in total permeate flow is approximately 0.4%. When comparing these results to those found in literature it is difficult to determine whether they are accurate as most major established plants and other experimental test rigs operate with feed water temperatures of approximately 25 oC, [10] resulting in no wasted energy through preheating or cooling the feed stream. An example of this is the SWRO plant in Qatar which operates at 25 oC producing 223.2 cubic meters of permeates daily between 500 and 1000ppm from a feed of 58,000ppm concentration [11]. Although a number of larger plants operate at the standard temperature of 25 oC, a year round study conducted in Tunisia [12] using a small scale domestic RO system found that higher feed water temperatures in the summer months resulted in up to 8% higher recovery rates for the small system. In saying this, it should be noted that the feed water in this study was supplied from natural sources and subject to limited pre-treatment (chemical free filtering for suspended solids) in which the salinity of the feed varied depending on the climatic conditions. pH levels also varied due to these conditions while Figures 4 and 5 assume constant feed properties.

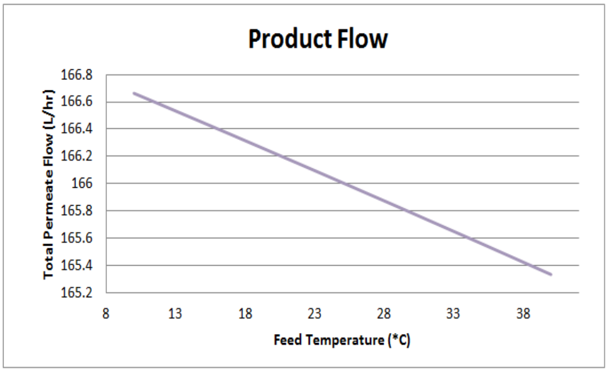

Figure 4: Total product flow against variable feed water temperature.

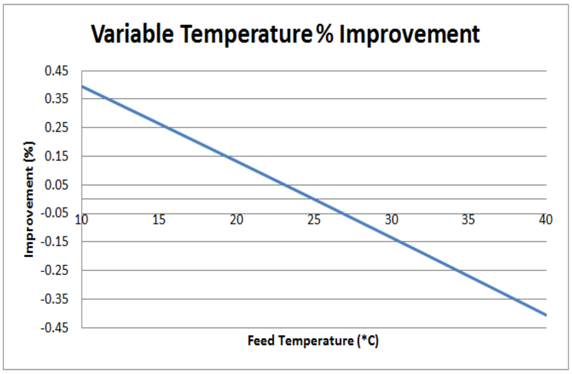

Figure 5: Percentage improvement for variable feed water temperature.

Pressure: Temperature of the feed water was returned to 25 °C for the pressure optimisation investigation with the flow rate remaining at the original 0.414 m^3/hr. The feed pressure was varied from 30 bar to 80 bar which in fact exceeds manufacturer's recommended maximum operating pressure by 14%. From the simulations it was found that the total product flow remained constant, along with the individual product stream concentrations which were seen to stay within the set boundary of 500ppm. This can be seen in Figure 6. Although the constant product stream concentrations were simulated beyond the maximum operating pressures outlined by the manufacturer, the output data shown in Figure 6 correspond to those shown in RO plants such as the Sharjah BWRO plant in United Arab Emirates where the concentration of each RO module remains constant in each arrangement pass as they are subjected to variable pressures [11]. The increase in feed pressure saw a directly proportional rise in the pressure of each brine steam, although the pressure drop in the membrane modules remained unchanged. This again resembles current plants in operation regardless of size or output capacity including Sharjah and Qatar [11] as there is a limited maximum pressure drop across each membrane during operation. With the increase in the brine pressure, an opportunity for the addition of multiple ERD's to the system is presented. Although the initial system requirements have been met, the initial power generated from the ERD devices can contribute to the funding of additional membranes to further increase the system efficiency and output. The brine stream pressures plotted in Figure 7 show the relationship between the increased feed pressure and the corresponding retentate pressure output. The feed pressure would only be able to increase to 6.9MPa due to maximum pressure limits specified by the manufacturer.

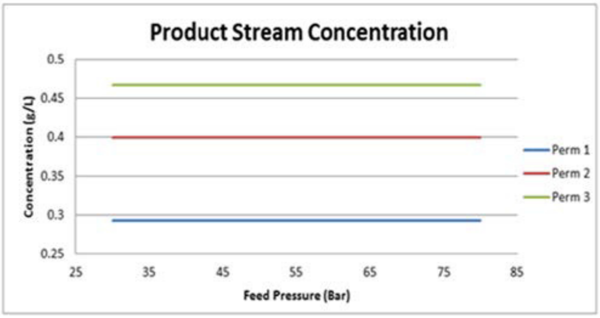

Figure 6: Product stream concentration with variable feed pressure

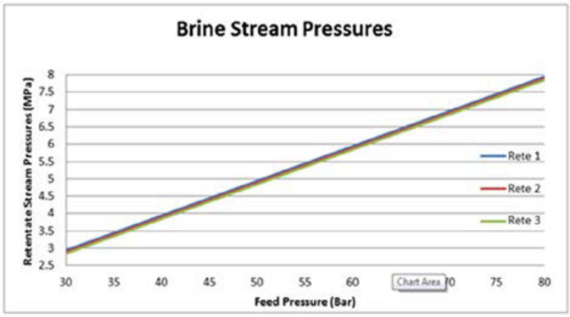

Figure 7: Brine stream pressure increase with variable feed pressure

*Feed Concentration :*As expected, the alteration of feed concentration had immediate and substantial impacts to the product flow and concentration of the retentate streams as shown in Figure 8. With temperature, pressure and feed flow established at 25 oC, 34.474 bar and 0.414 m3/hr, the product flow increased almost linearly as the feed concentration was decreased. As feed flow remains constant, a diluted feed diffuses more readily through the membrane as it has a constant salt rejection factor. Studies by both Majali et al. [11] and Elfil et al. [12] report that both large scale and small scale plants exhibit behaviors like those shown in Figure 8 where increased feed concentrations inhibit product flow levels. These reports and the relationship plotted in Figure 8 reflect the maximum membrane salt rejection properties which are outlined by the Hydranautics as being 99.4% for the SWC-2540 membrane used in the simulations. As the concentration of the feed water increases, the permeate flow reduces as the diffusion process through the first membrane under constant pressure is lengthened. Figure 9 shows this relationship graphically as the three permeate streams are plotted against the changing feed concentration.

As seen in Figure 9, the flow through the first and second membranes is up to 71.7% and 25.4% greater respectively, than those seen in the triple arrangement validation simulation. Once the stream passes through the third membrane, the flow rate returns almost to the initial flow rates as the salt concentration has again increased after the first two passes. Although increased flow rates are seen as a result of this investigation, it must be noted that the initial feed concentration of 35g/L was used to replicate the coastal water conditions of Central Queensland and specifically Yeppoon. Unless brackish water supplies of lower concentrations are to be used in the system, further pre-treatment is needed in order to alter the feed concentration conditions to replicate those in the above simulation.

*Feed Flow :*The variable feed flow optimizations simulation resulted in product flow data returns almost linearly proportional to the increase in the feed flow. With feed temperature and pressure at 25 oC and 34.474 bar respectively, the feed flow was altered from 0.05 m3/hr to 1.5 m3/hr in increments of 0.05 m3/hr. Permeate concentrates remained below the 500ppm limit for all flow rates which was expected as the feed concentration was again set to 35,000mg/L. Figure 10 shows the total product flow as the feed flow increments rose. As anticipated, the product flow increased as the system was subjected to a rising feed rate and exhibits behavior that reflects data found in a study by Majali et al [11] on both the Sharjah and Qatar RO plants. Figure 11 outlines the relationship found in this study between the feed and product flows at the Qatar SWRO plant which operates at a daily capacity of 223.5 m^3.

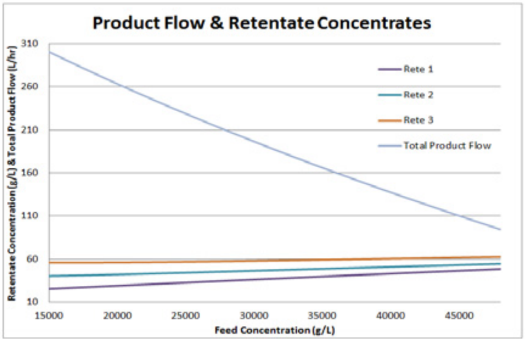

Figure 8: Product flow and retentate concentrates subject to variable feed concentration.

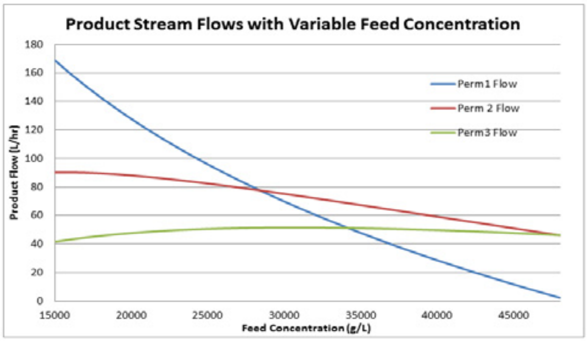

Figure 9: Product stream flows with variable feed concentration.

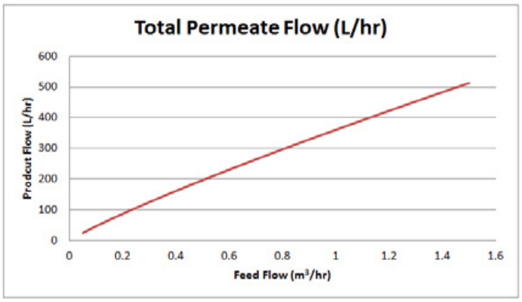

Figure 10: Total product flow with increasing feed flow.

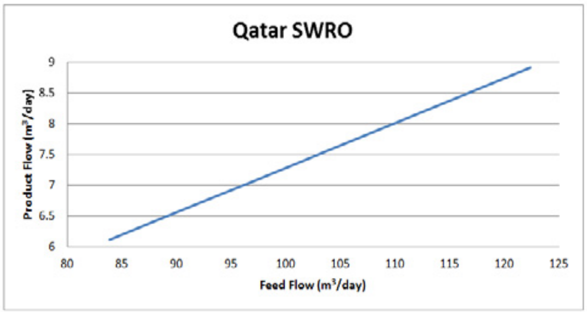

Figure 11: Feed & Product Flow relationship of the Qatar SWRO Plant (Majali et al. 2008).

Although Figure 12 suggests a relatively simple relationship between the two sets of data, an investigation into the water conversion factor (WCF) of the simulations, which relates to the system recovery, shows that at smaller flow rates, the system operates at greater efficiencies. Over the range of feed flows simulated, an increase in system efficiency of almost 15% can be seen. This efficiency relationship is plotted below in Figure 12. Comparison between Figures 10 and 12 present opportunities for a user to select the most efficient feed flow depending on the desired output of the system. Using the case of the validation data where 0.5 m3/day was required from a 6 hour operational day, the most efficient system feed can be found to be 0.109 m3/hr using the optimization data and a linear approximation through interpolation. The calculation of the most efficient and appreciate system arrangement also applies the assumption that the feed temperature and pressure remain constant at the values the optimization data was evaluated. In comparison to the other feed water characteristics of temperature, pressure and concentration, the feed flow is a variable that can be altered at no additional costs or variation to the system. This ensures the small scale solar desalination arrangement operates at the most efficient level whilst still providing the minimum desired output promoting longevity of the system components and most importantly the membranes.

4. Conclusions

The primary purpose of this study saw the development of a computational model to simulate and sequentially optimize the performance of a small scale solar desalination plant as a function of operating variables using Aspen Plus software. As a part of the project, an investigation into desalination indicated that solar RO desalination systems provide a sustainable solution to the increasing scarcity of fresh water sources especially in Australia where saltwater is an abundant resource. In comparison with a set of validation data, the simulated model was validated before optimizations simulation took place in order to improve current outputs.

Once the system was verified, optimization of the functional parameters was investigated providing results that both aligned with literature studies and current practice in operating RO plants around the world giving further evidence of system verification. Based on the results of the optimization phase, the impact of variable feed water characteristics were discussed, analyzed and compared, with feed flow concluded as the most cost effective and easily altered property for the small scale simulated system. By using the optimization results and the water conversion factor plot, the most efficient system can be obtained while desired outputs are still met.

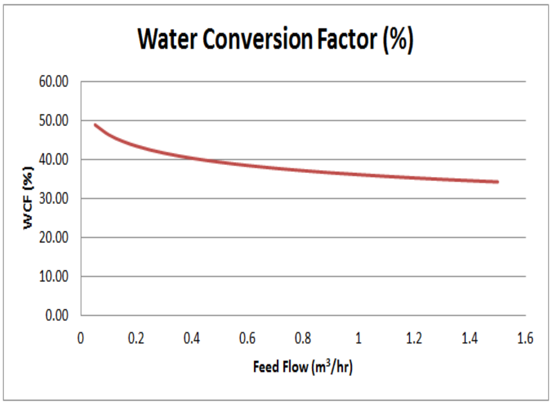

Figure 12: Water Conversion Factor for Variable Feed Flow Simulations.

Although it was found that additional changes to temperature, pressure or concentration of the feed-water can results in system improvements, feed flow was seen to be only variable that provides a seemingly cost free and instant improvement in system efficiency of up to 15%. Along with this enhancement it was also noted that the concentration of the permeate remained below the 500ppm limit meaning the product permeate remained within the potable range. Additionally, the variation of the feed flow provides the option to alter the desired output based on the level of potential solar energy each day.

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