MODELING AND COMPUTER SIMULATION OF REVERSE OSMOSIS SYSTEM FOR WATER TREATMENT

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ABSTRACT

Water represents the essence of life on earth, so we must preserve and use responsibly this given resource. For many years, water treatment has been a field of continuous development. At the same time, new materials and techniques are being developed for one of the most important methods in water treatment: Reverse Osmosis (RO).

Actual technology in this domain provided us with good know-how to reverse osmosis systems creation, simulation, and validation of the simulation results. Our duty is to bring value to this heritage with new specific cases where the known techniques will be used to create efficient models for water treatment by reverse osmosis.

Reverse osmosis is mainly a method for seawater desalination which started to be used more often in industrial applications for water and other product treatment.

The focus of this study is to design and simulate a reverse osmosis system with the help of Q+ Projection software v3.1 for a 10 m^3/h well water flow by using different types of membranes, in order to select an appropriate membrane which will provide the best parameters for permeate water.

Permeate water resulted after reverse osmosis treatment will be used as process water for spirit drinks production.

KEYWORDS: reverse osmosis, membrane, Q+ projection software, spirit drinks.

INTRODUCTION

Water represents one of the key needs for life on earth. During the years, the natural water resources started to be used more and more because of the industrial development and population growth. Freshwater resources are limited, so founding an alternative to produce freshwater became one important aspect. Together with the freshwater production, there is the wastewaters treatment, at the same level. The disposal of the wastewater in the environment without treatment will also reduce the freshwater volumes by contamination, in some cases.

To understand better the actual freshwater needs, "In a report tabled by Grail Research on the water availability per capita, India, China and most parts of Africa are predicted to face water shortages in the near future. Even countries in Central and Eastern Europe will face water shortage if immediate steps are not taken to conserve and minimize water usage", see Figure 1 [1].

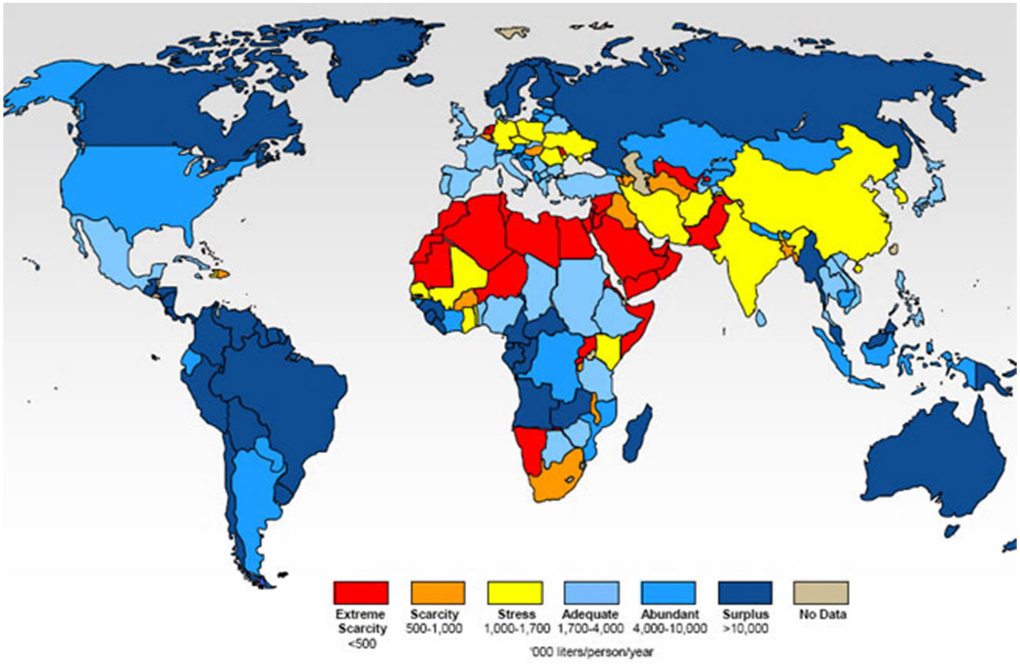


Figure 1. Global per capita water availability (2025) [1]

Figure 2 is presenting the distribution of the water in the world and over 96% is saline water in the oceans.

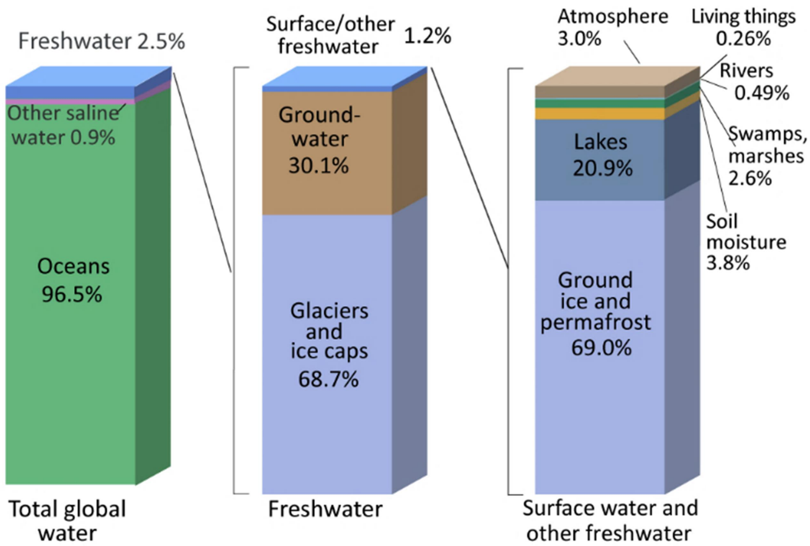


Figure 2. Distribution of the water in the world [2]

Oceans water resource is saline water and represents a huge resource that can assure the actual need for potable water. Actual technology includes several techniques for water desalination.

Water desalination is considered the main source of producing clean water from a variety of sources. Desalination refers to the process of removing the salts and minerals (contaminants) from either seawater or brackish water to obtain clean water suitable for human consumption and industrial and domestic usage [3].

The desalination technologies are grouped in two large families according their operating principle:

- thermal desalination processes that ensure a phase change of the solution to be desalinated, this phase change being done by freezing and distillation.
- membrane desalination processes, which represent a physical barrier to the separation of salt molecules from water. These separation techniques are grouped into three major classes according to the physical and chemical characteristics of membranes, the mode of operation or the driving force used to ensure separation: the filtration on the membrane, dialysis, and electro dialysis [4].

Reverse osmosis

Osmosis, in simplest terms, can be defined as a natural process in which water molecules spontaneously move from a solution of low solute concentration (low osmotic pressure) to a solution of high solute concentration (high osmotic pressure) across a semipermeable membrane (Figure 3a). The membrane, being semipermeable, rejects the solutes and only allows water molecules to pass through. The process of osmosis continues until a state of osmotic equilibrium is reached, when the chemical potentials across the membrane become equal (Figure 3b) [3].

The flow of water molecules can be stopped or reversed by the application of external pressure on the solution of higher concentration (feed solution). If the applied pressure difference is greater than the osmotic pressure difference across the membrane, water molecules are forced to flow in a direction opposite to that of the natural osmosis phenomenon. In such a case, the process occurring is known as reverse osmosis (RO) and is depicted in Figure 3c [3].

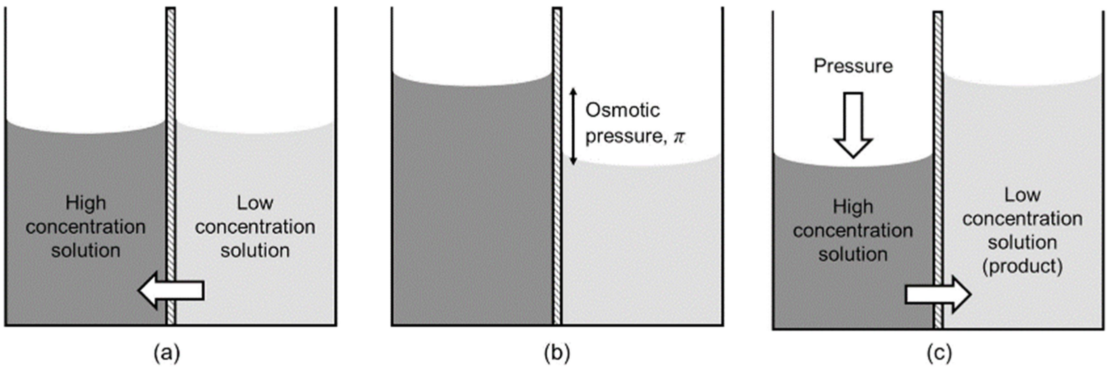


Figure 3. (a) Osmosis. (b) Equilibrium State. (c) Reverse osmosis [3]

In reverse osmosis systems can use different membrane types and modules such as: Figure 4a (plate and frame), Figure 4b (tubular), Figure 4c (spiral wound), and Figure 4d (hollow fiber).

The most used membranes in various applications are wraparound type (Figure 4c). These membranes are made of a flat membrane wrapped around a central perforated tube that collects the permeate.

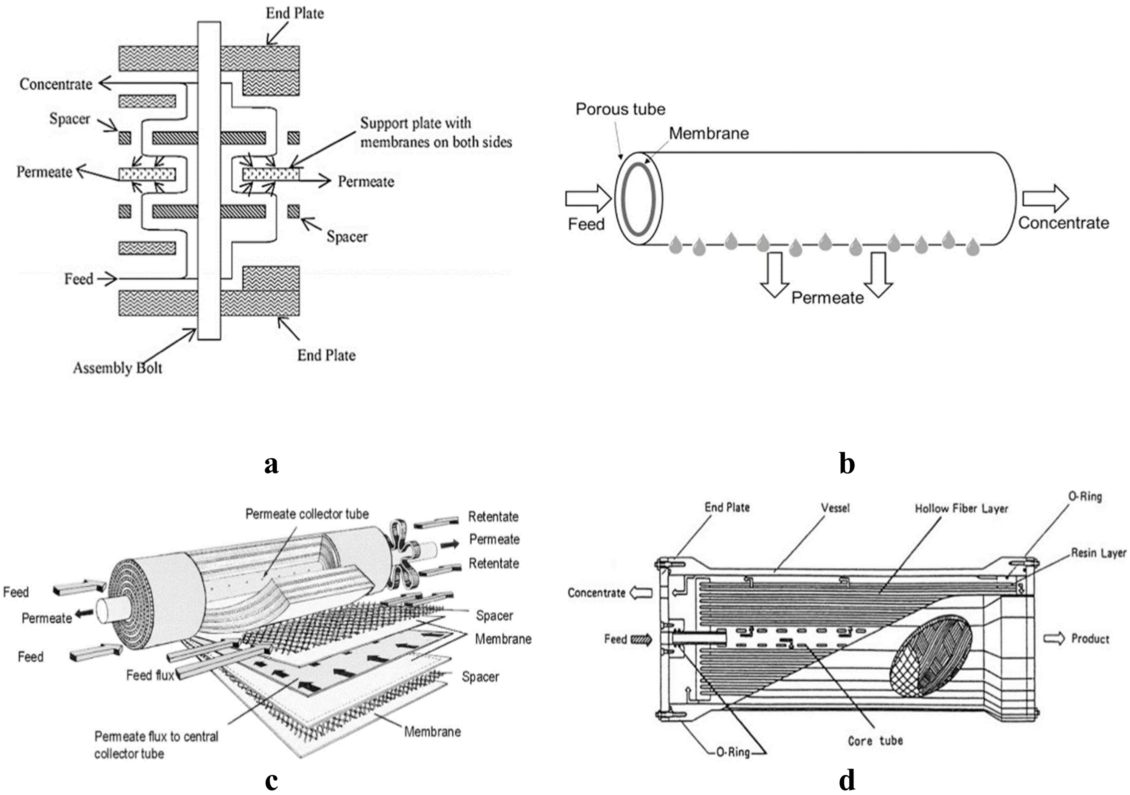


Figure 4 a. Plate and frame membrane module. b. Tubular membrane module. c. Spiral wound modules. d. Hollow fiber membrane module [3]

The membrane sheets are glued on three sides and the fourth one is connected to the central tube and it is open. The membrane leaves are then placed together with a feed/concentrate mesh spacer to induce turbulence and minimize the concentration polarization (CP) effects. The combination of leaves and feed/concentrate spacers is wrapped around the permeate collector tube to create a spiral configuration and finally placed inside a pressure vessel (also known as housing). Feed water is introduced from one end of the module and travels axially along the length of the module. Water molecules are forced through the membrane and are collected as permeate through the perforated permeate collector tube. The concentrate leaves the module at the end opposite to the feed [3].

The pressure vessels can be interconnected in different configurations to obtain a bigger membrane surface or better permeate quality. The membrane is semipermeable, and it is acting as a barrier for all contaminants and under pressure force allows only permeate water to pass; all contaminants are rejected as a concentrate which is collected from the pressure tube (membrane housing), see Figure 5.

Spiral wound modules are cost-effective, possess high packing density, and allow high mass transfer rates due to the presence of feed spacers. However, they are difficult to clean and are susceptible to fouling if pre-treatment is inadequate. In addition, spiral wound modules result in high feed side pressure drop. Commercial spiral wound RO membranes are available from manufacturers such as the Dow Chemical Company (Michigan, USA), Toray Membrane (California, USA), Koch Membrane Systems Inc. (Massachusetts, USA), and Suez Water Technologies (Pennsylvania, USA) [3].

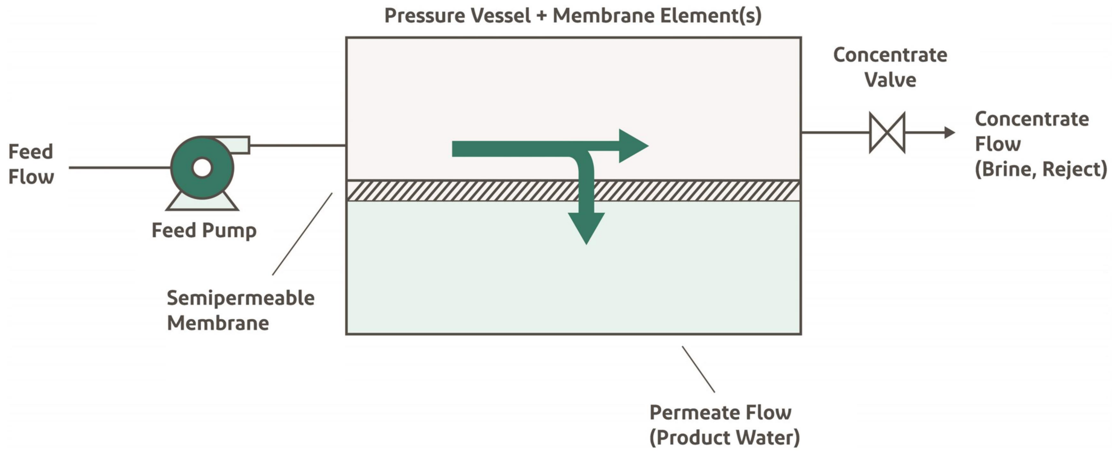


Figure 5 Reverse osmosis process [5]

Another top manufacturer for reverse osmosis membranes is LG Chem (Seoul, South Korea). LG Chem manufactures NanoH2O™ seawater and brackish water RO Membranes based on innovative Thin Film Nanocomposite (TFN) technology. Seawater RO Membranes provide industry-leading salt rejection (99.89%) [6].

Reverse osmosis system simulation

Water in spirit drinks production represents either a raw material or a product used in technological processes, such as cleaning. Water as raw material can be obtained through purification methods, such as reverse osmosis. The reverse osmosis in our case will separate all contaminants from well water, with the help of a semipermeable membrane to obtain high purity water, named permeate.

Spirit drink represents an alcoholic beverage, intended for human consumption, possessing particular organoleptic qualities, having a minimum alcoholic strength of 15 % vol., being produced either directly by distillation or by mixture [7].

Customers usually evaluate spirit drinks products mainly on organoleptic properties and aspect. To achieve better organoleptic properties, the purified water, and other ingredients such us ethylic alcohol quality are essential. For the best quality of most spirit drinks, producers use reverse osmosis systems with or without chemical dosing in feed water.

The following simulations show a model of simulation with the help of reverse osmosis projection software Q+ Projection v3.1 from LG Chem manufacturer, and how to select the most appropriate membrane type for a reverse osmosis system, which will assure the best permeate water quality in order to be used as raw material for spirit drinks production.

Some of the key parameters in permeate water used for spirit drinks are pH and TDS. These two parameters influence the organoleptic properties and aspect of the spirit drinks.

TDS concentration describes the presence of inorganic salts and small amounts of organic matter in water [8].

The TDS must be as small as possible because in spirit drinks inorganic salts and small amounts can generate deposits inside of the drinks, which will be visible in the bottle and can generate a bad appreciation from customers.

Next simulations for various conditions will be performed with Q+ Projection software version 3.1 from LG Chem manufacturer. During the process simulations at different recovery percent's the following factors will be evaluated: permeate pH, permeate TDS, feed pressure, and energy consumption.

Single-step simulation

First step in reverse osmosis systems simulations is the feed water analysis. The key parameters measured were feed water: pH, TDS (Total Dissolved Solid), and some specific chemical properties. The feed well water profile was created inside of the simulation software as per well water analysis, see Table 1.

Table 1 Feed water parameters for simulations

Total Disolved Solid (TDS)	1587.82	ppm	
Total Osmotic Pressure	1.05	bar	
pH	7.1		
Name	**ppm**	**ppm as $CaCO_3$**	**Balanced ppm**
Ammonium (NH4)	0.04	0.11	0.04
Sodium (Na)	557.93	1213.42	557.86
Potassium (K)	4.5	5.75	4.5
Magnesium (Mg)	0	0	0
Calcium (Ca)	0.1	0.25	0.1
Strontium (Sr)	0	0	0
Barium (Ba)	0	0	0
Fluoride (F)	0	0	0
Chloride (Cl)	610	860.37	610.07
Sulfate (SO_4)	85	88.49	85.01
Nitrate (NO_3)	25	20.16	25
Carbonate (CO_3)	0.31	0.52	0.18
Bicarbonate (HCO_3)	305.02	249.93	305.06
Boron (B)	0	0	0
Bromide (Br)	0	0	0
Silica (SiO_2)	0	0	0

Simulations will be done with: Q+ Projection software version 3.1, from LG Chem manufacturer on:

- seven identical membrane elements which are placed in the same pressure vessel.
- membrane elements selected as per next Table 2.
- a well water with: SDI (Silt Density Index) <3, pH 7.1 at 10°C Temperature.
- a feed flow of 10 m^3/h.
- water parameters described in Table 1.

A graphic representation of one reverse osmosis system design is shown in Figure 6 (capture from Q+ Projection software).

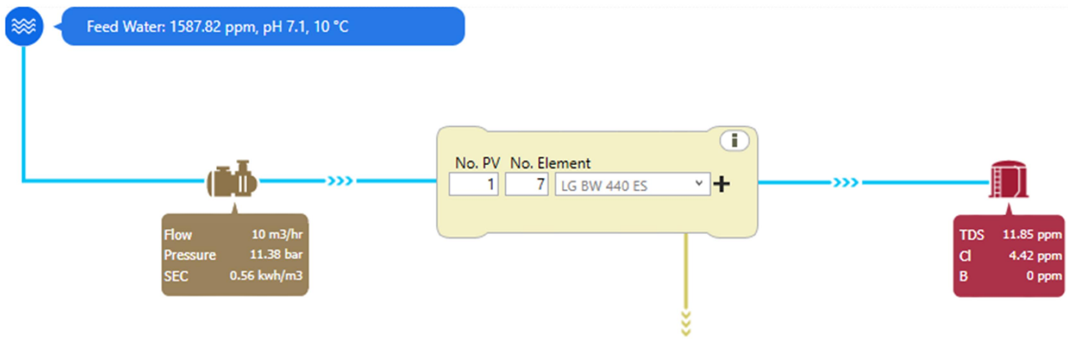


Figure 6. Graphic representation for RO system design

The selection of membrane elements for these simulations was based on membranes' properties and manufacturer recommendations, for food and beverages application, see Table 2.

Table 2. Selected membranes for simulations

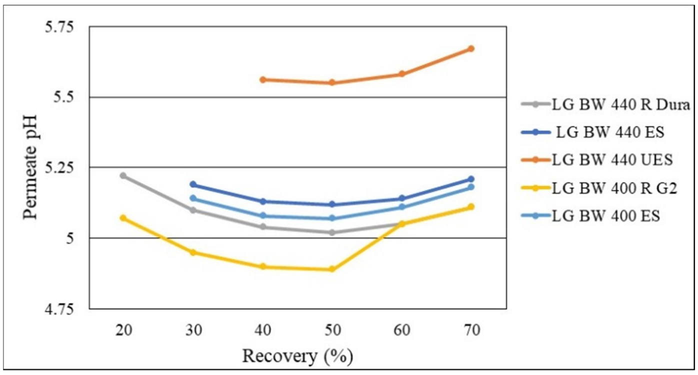
Membrane name	Membrane type	Active Membrane Area	Permeate Flow Rate
LG BW 440 R Dura	High Rejection, High Durability	41 m^2	43.7 m^3/d
LG BW 440 ES	Energy Saving	41 m^2	43.7 m^3/d
LG BW 440 UES	Ultra Low Energy	41 m^2	47.9 m^3/d
LG BW 400 R G2	Anti-Fouling, Superior Rejection, High Flow, High Durability	37 m^2	43.5 m^3/d
LG BW 400 ES	Energy Saving	37 m^2	39.7 m^3/d

All the five types of membranes were simulated under the same conditions, described above at different recovery rates, starting from 20% up to 70% (which corresponds to a permeate flow of 2 up to 7 m^3/h).

In spirit drinks, water is very important and contributes to the texture and organoleptic properties of the drinks.

In our study for permeate water obtained after reverse osmosis treatment, we intend to obtain a pH of 5.2-5.5 and a TDS of 5-12 mg/L, permeate that can be used for spirit drinks production as raw material. In simulations, we aim to analyze the influence of these membrane types on permeate water parameters, without neglecting energy consumption.

The results on key parameters (permeate pH, permeate TDS, feed pressure, and energy consumption) after simulation on each membrane type are compared in Figure 7.



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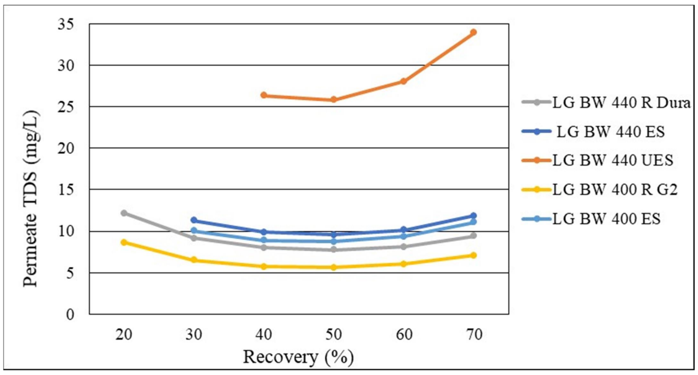

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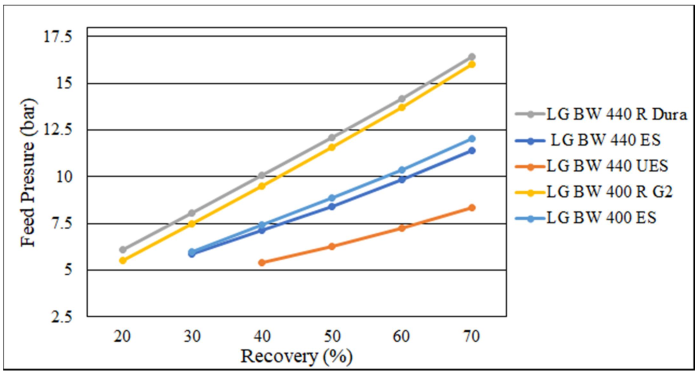

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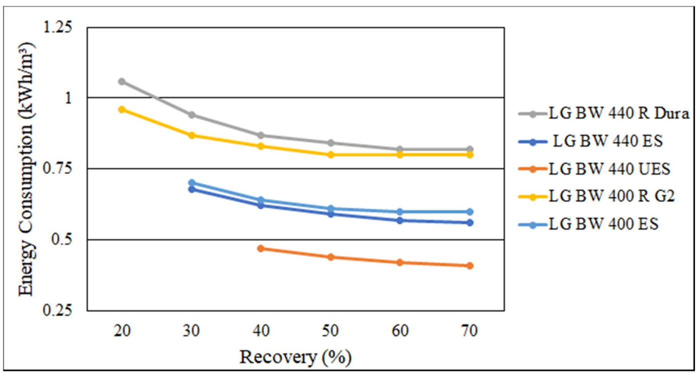


d

Figure 7 Results after simulation of selected membranes: a. Permeate pH results, b. Permeate TDS results, c. Feed pressure results, d. Energy consumption results.

The permeate pH, permeate TDS, and feed pressure trend is to increase at a higher recovery rate; at the same time, the energy consumption trend is to decrease at higher recovery rate. It is observed from Figure 7a and Figure 7b that permeate pH and TDS are outside the limits for LG BW 440 UES membrane (pH above 5.5 and TDS above 25) and for LG BW 400 R G2 the pH is below 5. Therefore, these two membranes can be excluded, although the LG BW 440 UES would ensure the lowest power consumption, see Figure 7d.

For the LG BW 400 R G2 and LG BW 440 R Dura membranes, Figure 7c and Figure 7d show at 60-70% recovery (permeate flows of 6-7 m^3/h) that the pressures of the feed water flow are 14-16 bar which leads to higher energy consumption; based on this, these membranes can be excluded from our study.

By analyzing all the simulation results from Figure 7 we can observe that LG BW 440 ES & LG BW 400 ES membranes are the most stable from all five-membranes evaluated.

Table 2 shows the LG BW 440 ES & LG BW 400 ES membranes characteristics on active membrane area and industrial permeate flow. From this Table 2, we can observe that LG BW 440 ES has a bigger transfer surface area and permeate flow rate.

Finally, a summary of our results for all five membranes is shown in Table 3.

Table 3. Simulation results for selected membrane types at 70% recovery (7 m^3/h permeate flowrate)

Membrane type	Permeate pH	Permeate TDS (mg/l)	Feed Pressure (bar)	Energy consumption (kWh/m^3)
LG BW 400 R G2	5.11	7.08	16.04	0.8
LG BW 440 R Dura	5.11	9.39	16.44	0.82
LG BW 400 ES	5.18	11.07	12.07	0.6
LG BW 440 ES	5.21	11.85	11.38	0.56
LG BW 440 UES	5.67	33.9	8.36	0.41

The results in Table 3 show that the performance of LG BW 440 ES membrane at 70% recovery during our simulations is the most centered pH from these simulations, with less TDS, high feed flow and reduced energy consumption, too. Therefore, all these results indicate the possibility of using the LG BW 440 ES membrane in the spirit drinks industry.

But the design process is not completed only after a few simulations. Selected membrane type in our case LG BE 440 ES should be simulated in different conditions which need to include the worst conditions that can occur.

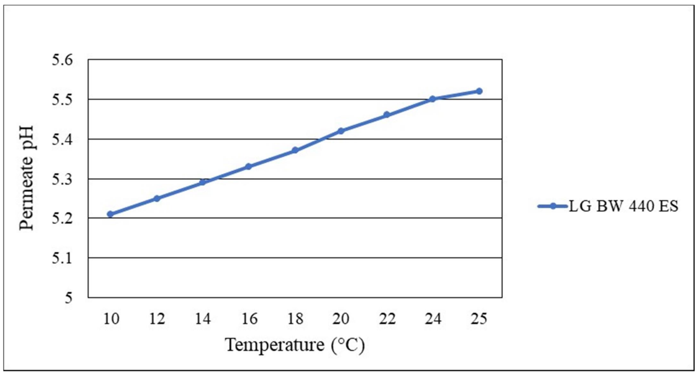
Simulation of RO membrane factors

To define the worst conditions, three RO membrane influence factors: feed water temperature, feed water pH, and membrane aging, will be simulated within extreme values. For the definition of extreme values, few simulations will be done to show the effect of these influence factors.

Feed water temperature influence

This simulation is made for the same feed water parameters defined in Table 1, with the same feed flow of $10 m^3/h$ of well water type (SDI<3) at 0 years membrane age. The range of temperature was established between 10 and 25 °C and feed water pH is 7.1.

The results of temperature simulations show that the lowest temperature is generating the lowest permeate pH and TDS values, see Figure 8. But, to obtain a permeate pH between 5.2 and 5.5 and a TDS between 5 and 12, the supply temperature of 11-12 °C cannot be exceeded.



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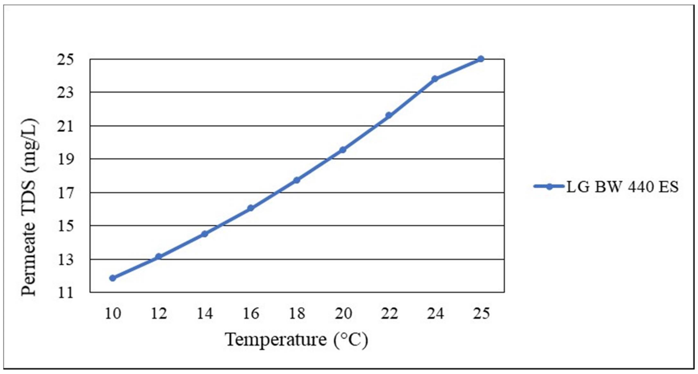

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Figure 8. Feed water temperature effects on:
a. permeate pH b. permeate TDS

Feed water pH influence

This simulation is made for the same feed flow of $10 m^3/h$ of well water (SDI<3) with water parameters as per Table 1 at 0 years membrane age and lowest feed water temperature (10°C).

The results of this pH simulation show us that the highest feed water pH generates the highest permeate TDS values, as can be seen in Figure 9. At feed water pH over 7.4, the permeate exceeds the targeted permeate TDS established at 12. So, for LG BW 440 ES membrane design reverse osmosis process, the feed flow pH must be limited under 7.4.

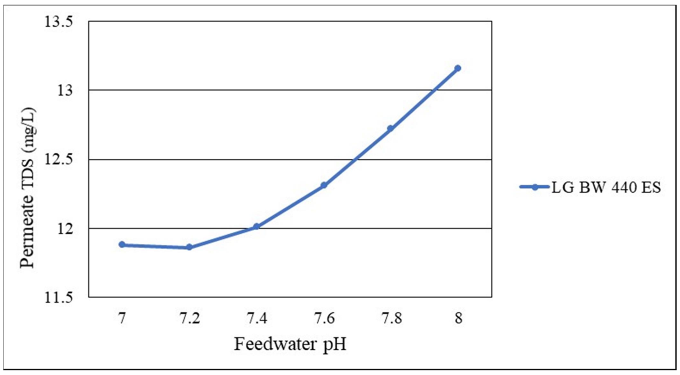
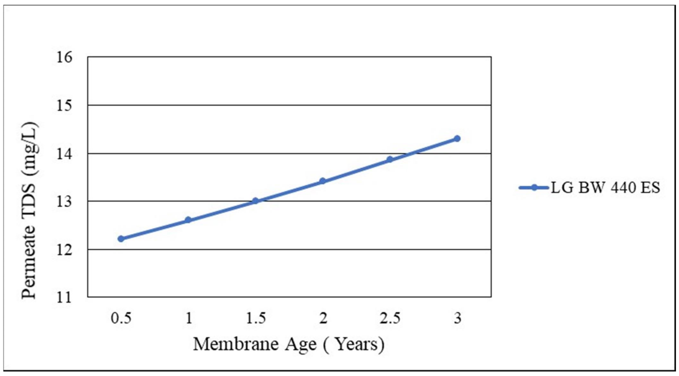


Figure 9 Feedwater pH influence on permeate TDS

RO membrane aging simulation

This simulation is made for the same feed water parameters defined in Table 1, with the same feed flow of 10m^3/h of well water type (SDI<3) at different membrane age. The feed water temperature was established at 10°C with a pH of 7.1. The results are showing that the membrane aging is increasing the TDS and feed water pressure, see Figure 10.

Figure 10a shows that a TDS value of 12-12.5 mg/l can be maintained only if LG BE 440 ES membrane cleaning will be done every 6 months of RO system operation. Membrane aging is also reflected in the increase of the feed pressure due to the membrane fouling, see Figure 10b.



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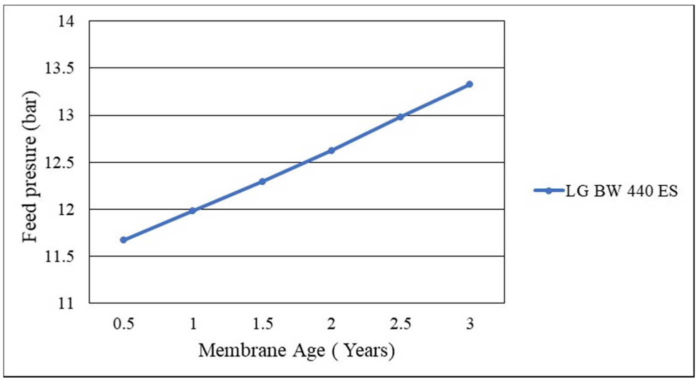

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Figure 10 Membrane age effect on: a. permeate TDS, b. Feed pressure

During this step of the simulation, we have noticed that different pH values on feed water did not have a significant impact on feed pressure and energy consumption, the results on these being almost linear (results not given in this paper).

Worst RO membrane conditions simulations

As observed in Figure 9, for LG BW 440 ES membrane, the feed water pH must be kept below 7.4 in order not to affect the targeted permeate pH and TDS. Starting from the feed water temperature of 12 °C and pH 7.4, a series of 5 simulations were performed on the selected membrane LG BW 440 ES, considering its operation for 2 years. Based on the above results, which show that increased feed water temperature, pH and higher membrane aging are increasing the permeate pH and TDS values, we have defined as worst conditions those given in Table 4. In the same Table 4, we have also added initial simulation and system design data, together with simulation of initial conditions at 0.5 years membrane age.

Table 4. Worst condition for reverse osmosis system simulation and results

Input		**Initial conditions**		**Worst conditions**				
		Initial	**Initial 0.5 years**	**# 1**	**# 2**	**# 3**	**# 4**	**# 5**
Water Type	-	Test Water	Test Water	Test Water	Test Water	Test Water	Test Water	Test Water
Feed TDS	ppm	1587.82	1587.82	1587.82	1587.82	1587.82	1587.82	1587.82
Temp	°C	10	10	12	12	12	12	12
pH	-	7.1	7.1	7.4	7.4	7.4	7.4	7.4
Years of operation	-	0	0.5	0	0.5	1	1.5	2
Feed	m^3/h	10	10	10	10	10	10	10
Recovery	-	70 %	70 %	70 %	70 %	70 %	70 %	70 %
Design								
Stage		Stage 1	Stage 1	Stage 1	Stage 1	Stage 1	Stage 1	Stage 1
Membrane		LG BW 440 ES	LG BW 440 ES	LG BW 440 ES	LG BW 440 ES	LG BW 440 ES	LG BW 440 ES	LG BW 440 ES
# Pressure Vasel (PV) per Stage		1	1	1	1	1	1	1
# Element per PV		7	7	7	7	7	7	7
Output								
TDS	ppm	11.85	12.22	13.3	13.71	14.14	14.58	15.04
pH		5.21	5.22	5.52	5.53	5.55	5.56	5.58
Feed Pressure	bar	11.38	11.67	10.73	11	11.28	11.57	11.88
Energy Consumption	kWh/m^3	0.56	0.58	0.53	0.55	0.56	0.57	0.59
Fouling factor	kWh/m^3	1	0.96	1	0.96	0.93	0.9	0.86

The increase of reverse osmosis process operation time (membrane aging) generates a feed flow pressure and energy consumption growth. Both permeate water quality decrease and energy consumption increase are results of membrane fouling, reflected by fooling factor, see Table 4. Fooling factor decreases from 1 at the commissioning of the process to 0.86 after 2 years of operation. The above worst condition # 5 is the worst one based on permeate pH and TDS values obtained.

Finally, the selected membrane type LG BW 440 ES is suitable to obtain a permeate flow of 7 m^3/h with pH 5.21 and 11.85 TDS with an input of $10m^3/h$ feed water flow at 10 °C and parameters per Table 1.

Because the reverse osmosis system performance will gradually decrease, after two years of operation in the worst conditions a permeate with 5.58 pH and 15.04 TDS can be obtained. These values no longer satisfy the established permeate water pH and TDS quality for spirit drinks production, so it is recommended to clean the membranes every 6 months in order to return them, as much as possible, to the initial state, and to ensure the desired permeate pH and TDS values.

CONCLUSIONS

This study presents a proposal for the design and simulation of a reverse osmosis system on a software, to select the appropriate membrane type for the best permeate to be used in spirit drinks production. The feed water used was a well water with the following characteristics: 7.1 pH, 10°C temperature, 1587 mg/l TDS, $10m^3/h$ flow, and it was simulated on a reverse osmosis system with Q+ Projection software version 3.1. The initial simulations were done on a single pass reverse osmosis system with one pressure vessel which contains seven identical membrane modules. Five different types of membranes modules (LG BW 400 R G2, LG BW 440 R Dura, LG BW 400 ES, LG BW 440 ES & LG BW 440 UES) were simulated and during simulations were tracked the influence of recovery on permeate pH and TDS, energy consumption and feed pressure. After this initial set of simulations, the membranes LG BW 440 UES and LG BW 400 R G2 showed that permeate pH does not satisfy the target values of pH (5.2-5.5) and TDS (5-12 mg/l) established as targets for this study. Also, in the same set of simulations the influence of recovery on feed water pressure and energy consumption were tracked. By tracking these two parameters we have seen that membranes LG BW 400 R G2 and LG BW 440 R Dura at higher recovery rate (70%) have a big feed pressure and energy consumption. From the remained two membranes, LG BW 440 ES and LG BW 400 ES, based on their characteristics (Table 2) we have seen that the former membrane LG BW 440 ES has a bigger active membrane area and permeate flow rate. Based on the above considerations the LG BW 440 ES membrane it was selected for next simulations. With this selected membrane and in initial conditions for feed water it was simulated the influence of feed water temperature, feed water pH, and membrane aging over permeate. From these simulations, we have seen that a pH over 7.4 and a temperature over 12 °C will generate a TDS over our targeted values for spirit drinks industry. By analyzing the membrane fooling factor at different membrane ages, we have also seen that membrane LG BW 440 ES requires a regular cleaning every 6 months. In order to confirm this fact, we have simulated the LG BW 440 ES membrane in worst condition that can occur: feed water with 7.4 pH, TDS 1587, temperature at 12 °C and membrane aging from 0 up to 2 years.

Finally, the simulation shows that LG BW 440 ES membrane should be regularly cleaned on a stream of maximum 0.5 years to keep the desired permeate parameters. In the end, we can say that the selected membrane type LG BW 440 ES is suitable for the production of a permeate flow of 7 m3/h (70% recovery) with pH 5.22 and TDS 11.67 with an input $10 m^3/h$ feed water flow at 10 °C with pH 7.1 and parameters per Table 1, paying attention to membrane cleaning at every 0.5 years of reverse osmosis system functioning. The permeate water thus obtained can be used in the spirit drinks industry.

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