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**MATHEMATICAL MODELING AND SIMULATION
OF A HEAT PUMP WATER DESALINATION PROCESS**

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(good afternoon)

1. INTRODUCTION

Numerous communities in the World and in Brazil show a lack of drinking water.

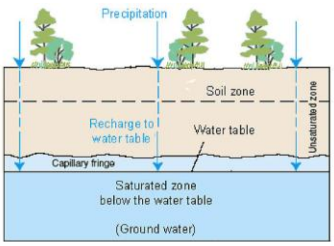

África


Brazil


África

In counterpoint to this reality, there are abundant sources available such as seawater and groundwater.

África



Ground Water

Brazil

Sea Water

África

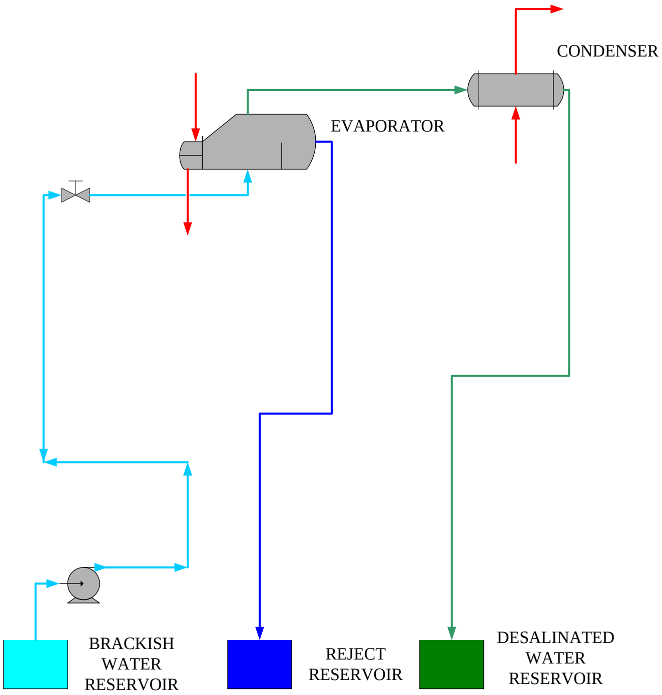
However, seawater contains about 3% of dissolved salts, and ground water may also be salted.

Thus, since 1960 drinking water is being obtained on a large scale by desalting through two main alternatives: membranes or evaporation (distillation), at a cost in 2001, which in some cases was less than US$ 0.70/m^3 drinking water produced. (Ettouney and El-Dessouky, 2001)
In 2005 the installed desalination capacity was estimated at 53.69 x 10^6 m^3 per day and the cost of treatment has come close to conventional prices, even in countries with no lack of water resources. (Reddy and Ghaffour, 2007)

MSF Desalination plant
23,500 ton/day x 20 units = total 470,000 ton/day
Al Jubail, Saudi Arabia.

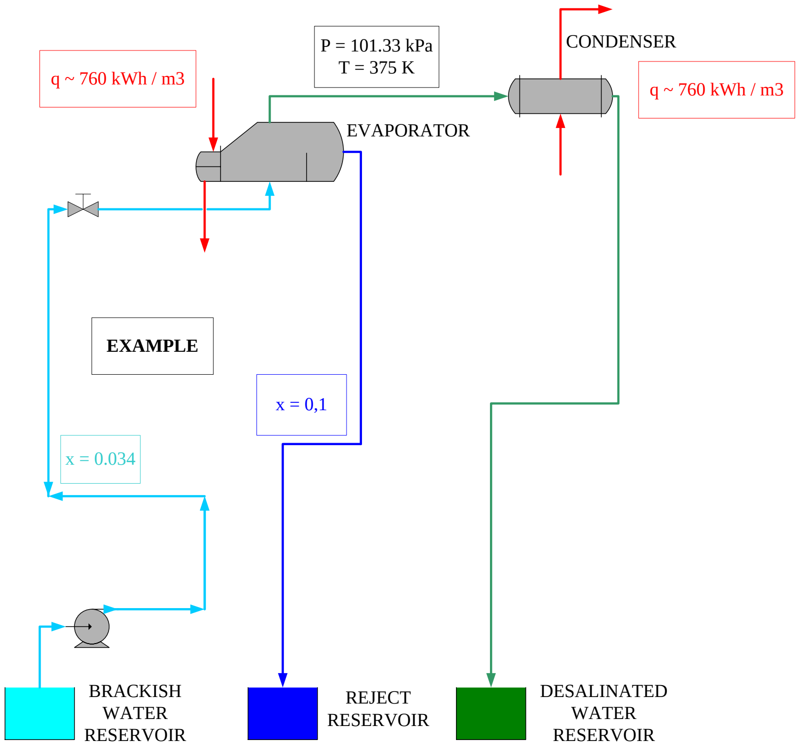
MSF Desalination plant
100 million ton/year
Shoaiba power and desalination plant, Saudi Arabia.

The simplest method of obtaining potable water by evaporation it is evaporation in a single stage, basically consisting of one evaporator and one condenser.

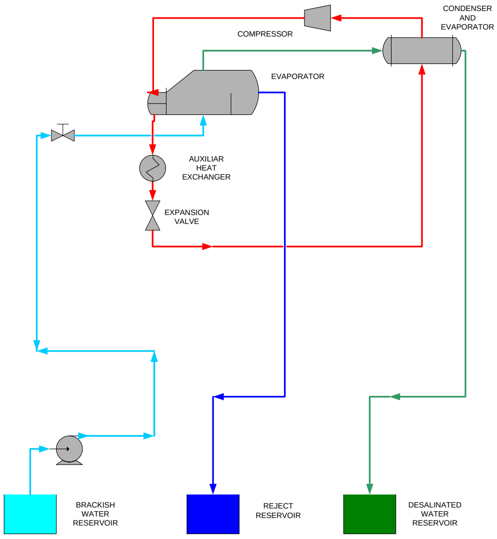


The salt water evaporates, producing steam which is then condensed. The residual salt water coming from the evaporator returns to the source.
However this is also the alternative that consumes the greatest amount of energy.

In the numerical example below, for desalination of sea water via this simpler alternative, the power consumption in the evaporation will be about 760 kWh / m^3 of fresh water produced. A similar amount of energy must be removed by condensation.



By definition, heat pumps are systems that promote the heat transfer from a low temperature region to another at higher temperature. (International Energy Agency, Heat Pump Programme, 2012)
In this work we employ a heat pump by Vapor Compression.



The evaporator of the seawater is also the condenser of the working fluid. The condenser of the drinking water is also the evaporator of the working fluid. At the heat pump, the energy received on the condenser, and on the compressor, must be the same to the energy removed. The auxiliary heat exchanger guarantees that. The working fluid is also pure water (R-718).

To further reduce the energy consumption, it was necessary to lower the temperature of the drinking water produced and also lower the temperature of the waste, avoiding thermal pollution. For that additional heat exchangers were added to the system.

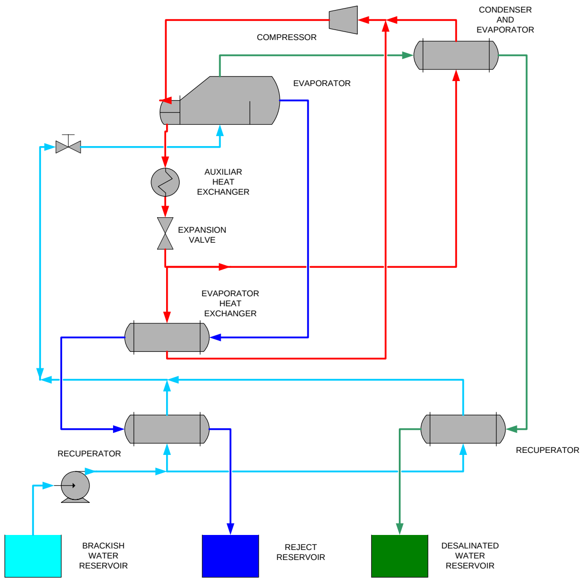


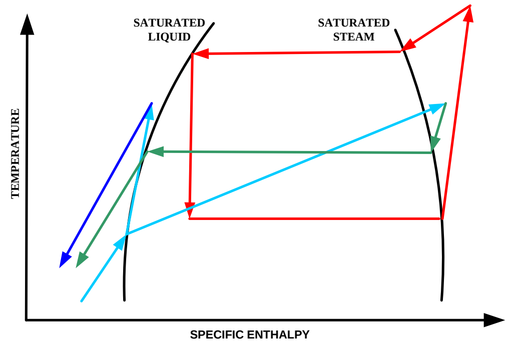
Figure 1. Desalination system proposed.

Salt water is preheated by cooling the waste and drinking water. The waste also contributes to evaporate part of the working fluid.

The objective of this work is to model this system for obtaining drinking water from brackish or sea water, through a heat pump, with mechanical compression of auxiliary fluid. Such system may be considered ideal for meeting the needs of small communities, even those that lack of highly qualified workers.

2. METHODOLOGY

The methodology used covers the techniques of material and energy balances associated with thermodynamic predictions. These, among other parameters, show the relation between impure water processed and desalinated water produced, as well as the power consumption of the proposed facility.
The general diagram specific enthalpy x temperature for the system is as follows.



3. MODELING ON STEADY OPERATION

The mass flow of saline water fed to the system, its concentration and the final concentration for the waste were considered independent variables.
Other variables arbitrarily set for the simulations were the differences in temperature between the fluids circulating inside the heat exchangers and the thermodynamic efficiency of the compressor.
The salt water was considered as having 0.002 kg of salt / kg and sea water 0.034 kg of salt/ kg.
High salt concentrations in the waste are avoided in the usual processing practice to eliminate or minimize fouling.
The temperature differences of the fluids on outputs in all heat exchangers were fixed at most simulations as 5 K.
Of all simulations, none show the pressure within the evaporator exceeding 200 kPa.

The complete mathematical modeling can be obtained with the authors. There are some copies available here for those attending this presentation.

MATHEMATICAL MODELING

The temperatures of the streams of waste and product were determined arbitrarily as that for saturation, corresponding to the working pressure in the evaporator. For the operability of heat exchangers, independent of the compression cycle, the temperature of the water supplied and already preheated must be fixed slightly below this value. In this work we adopted a reduction of 5 ° C.

$$T_6 = Tsat_8 - 5 \qquad (01)$$

The mass flow of saline water fed to the system, its concentration and the final concentration set for the reject are considered independent variables. The brackish water was considered as having 2,000 ppm salt and sea water 34,000 ppm. The material balance equations around the evaporator, determine the production of pure water and waste in the studied system.

$$F_7 = \frac{F_6 . x_6}{x_7} \qquad (02)$$

$$F_8 = F_6 - F_7 \qquad (03)$$

The operating pressure of the evaporator is another independent variable in the modeling. The operating temperature is given by equation (04)

$$T_8 = T_7 = Tsat_8 + epe_7 \qquad (04)$$

The amount of heat that must be provided by the compression cycle in the evaporator for the desired output is given by:

$$qEVA = F_7.h_7 + F_8.h_8 - F_6.h_6 \tag{05}$$

The amount of heat received by compression cycle through the heat exchangers thanks to the use of heat coming from the cooling of the product and reject can be estimated using equations (06) and (07).

$$qTC2 = F_7.(h_7 - h_9) \tag{06}$$

$$qTC3 = F_8.(h_8 - h_{10}) \tag{07}$$

The amount of heat received for feed preheating, is given by:

$$qTC4 + qTC5 = F_1.(h_6 - h_1) \tag{08}$$

To enable heat transfer in the evaporator, the temperature of the circulating fluid in the compression cycle must always be greater than the boiling temperature of the water in this equipment. In most cases the temperature difference was arbitrarily set to 5 ° C.

$$T_{13} = T_8 + dte \tag{09}$$

The expansion in the valve is considered to be adiabatic so that:

$$h_{13} = h_{14} \tag{10}$$

To make possible the heat transfer in heat exchangers, the temperature of the circulating fluid in evaporation should be smaller than the product and reject. The fixed temperature difference in the majority of the simulations was 5 ° C.

$$Tsat_{14} = Tsat_8 - dte \tag{11}$$

The heat released in the heat exchangers is absorbed by the fluid circulating in the vapor compression cycle. The following equation allow us to calculate the mass flow rate of fluid.

$$qTC2 + qTC3 = m.(h_{19} - h_{14}) \tag{12}$$

In an ideal compression, entropy remains constant.

$$sid_{20} = s_{19} \tag{13}$$

To provide the non-ideality of compression, with a consequent increase in entropy, it can be introduced in the equations the thermodynamic efficiency of the compressor (R).

$$R = \frac{hid_{20} - h_{19}}{h_{20} - h_{19}} \tag{14}$$

The energy consumption of the plant in kWh/m^3 pure water produced is directly related to the enthalpy variation within the compressor.

$$CON = \frac{(h_{20} - h_{19}).m.1000}{F_8.3600} \tag{15}$$

The calculation of excess energy (q) to be removed, can be made by:

$$q = m.(h_{20} - h_{19}) \tag{16}$$

The outlet temperatures of the waste and the product can be determined by calculation of enthalpies (h11) and (h12) by expression (17)

$$qTC4 + qTC5) = F_7.(h_9 - h_{11}) + F_8.(h_{10} - h_{12}) \tag{17}$$

The production capacity of the plant is given by:

$$PROD = {}^{F_8}\!/_{F_1} \tag{18}$$

PROPERTIES OF SALT SOLUTIONS AND PURE WATER

In the present work we use pure water as the circulating fluid in the vapor compression cycle. ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc.), calls that for such use as R-718 fluid. The heat capacity at constant pressure of the aqueous salt solutions and pure water (doing x = 0) in kJ / kg.K is given by El-Dessouky et al. (2000) where the temperature is in ° C and the concentration in kg / kg total. (equation 19)

$$cp = \left[aa. + bb.T + cc.T^2 + dd.T^3\right].10^{-3} \tag{19}$$

$$aa = 4206{,}8 - 6{,}6197.\left(\frac{x}{10^{-3}}\right) + 1{,}2288.10^{-2}.\left(\frac{x}{10^{-3}}\right)^2 \tag{20}$$

$$bb = -1{,}1262 + 5{,}4178.10^{-2}.\left(\frac{x}{10^{-3}}\right) - 2{,}2719.10^{-4}\left(\frac{x}{10^{-3}}\right)^2 \tag{21}$$

$$cc = 1{,}2026.10^{-2} - 5{,}3566.10^{-4}.\left(\frac{x}{10^{-3}}\right) + 1{,}8906.10^{-6}.\left(\frac{x}{10^{-3}}\right)^2 \tag{22}$$

$$dd = 6{,}8777.10^{-7} + 1{,}517.10^{-6}.\left(\frac{x}{10^{-3}}\right) - 4{,}4268.10^{-9}.\left(\frac{x}{10^{-3}}\right)^2 \tag{23}$$

The specific enthalpy of aqueous solutions or pure water may be calculated by:

$$h = \left[ll.(TK - TK0) + \frac{mm.(TK^2 - TK0^2)}{2} + \frac{nn(TK^3 - TK0^3)}{3} + \frac{dd.(TK^4 - TK0^4)}{4}\right].10^{-3} \tag{24}$$

Where temperatures are in K and the reference temperature is TK0 = 273.15 C. The other constants are:

$$ll = aa - bb.TK0 + cc.TKO^2 - dd.TKO^3 \tag{25}$$

$$mm = bb - 2.cc.TK0 + 3.dd.TK0^2 \tag{26}$$

$$nn = cc - 3.dd.TK0 \tag{27}$$

The conversion from degrees Celsius to Kelvin is the usual. The relationship between the saturation temperature and pressure, as well as latent heat of vaporization and saturation temperature are given below.

$$Tsat = TKsat - 273{,}15 \tag{28}$$

$$TKsat = 46{,}13 + \frac{3816{,}44}{16{,}2886 - \ln P} \tag{29}$$

$$hfg = 2256{,}1.\left(\frac{1 - TKsat / 647{,}3}{1 - 373{,}15 / 647{,}3}\right)^{0{,}325} \tag{30}$$

The heat involved on the overheating of the steam, depends on the temperature at which it lies and on the saturation temperature for pure water at the pressure considered. The specific enthalpy is given by:

$$h\sup = \left[a.(TK - TKsat) + \frac{b.(TK^2 - TKsat^2)}{2} + \frac{c.(TK^3 - TKsat^3)}{3} + \frac{d.(TK^4 - TKsat^4)}{4}\right].\frac{1}{18{,}016} \tag{31}$$

$$a = 33{,}46 \tag{32}$$

$$b = 0{,}688.10^{-2} \tag{33}$$

$$c = 0{,}7604.10^{-5} \tag{34}$$

$$d = -3{,}593.10^{-9} \tag{35}$$

The expression for determining the boiling point elevation of a salt solution depends on the concentration and temperature of solution and it is given by El-Dessouky et al. (2000).

$$epe = \left(\frac{x}{10^{-6}}\right).\left[ee + ff.\left(\frac{x}{10^{-6}}\right)\right].10^{-3} \tag{36}$$

$$ee = \left(6{,}71 + 6{,}34.10^{-2}.Tsat + 9{,}74.10^{-5}.Tsat^2\right).10^{-3} \tag{37}$$

$$ff = \left(22{,}238 + 9{,}59.10^{-3}.Tsat + 9{,}42.10^{-5}.Tsat^2\right).10^{-8} \tag{38}$$

20,000 < x < 160,000 and 20 ^{o}C < T < 180 ^{o}C

Unless better understanding, below 20,000 ppm concentration of salts in the water, the boiling point elevation is so low (bpe < 0.5 ° C) that not practical problems arise with the extrapolation of the lower limit of validity of the concentration for the equation submitted.

The total enthalpy and the total entropy of a superheated steam are given by the expressions (39) and (40)

$$h = hf + hfg + h\sup \tag{39}$$

$$s = sf + sfg + s\sup = sg + s\sup \tag{40}$$

The entropies were estimated by the expressions:

$$sf = [ll.\ln\left(TKsat/TK0\right) + mm.(TKsat - TK0) +$$

$$+ nn.(TKsat^2 - TK0^2)/2 + dd.(TKsat^3 - TK0^3)/3].10^{-3} \tag{41}$$

$$sfg = \frac{hfg}{TKsat} \tag{42}$$

$$s\sup = [a.\ln\left(\frac{TK}{TKsat}\right) + b.(TK - TKsat) +$$

$$+ c.(TK^2 - TKsat^2)/2 + d.(TK^3 - TKsat^3)/3].\frac{1}{18{,}016} \tag{43}$$

4. RESULTS

Rising the surrounding temperature decreases the size of the heat exchangers for preheating the feed, increases the temperature of the disposal of waste and purified water required and under the conditions of the proposed system does not change the power consumption of the installation.
Figures 2 and 3 present a summary of the results.
The compressor thermodynamic efficiency was defined as

efficiency = Variation on isentropic process enthalpy / enthalpy variation on the actual process

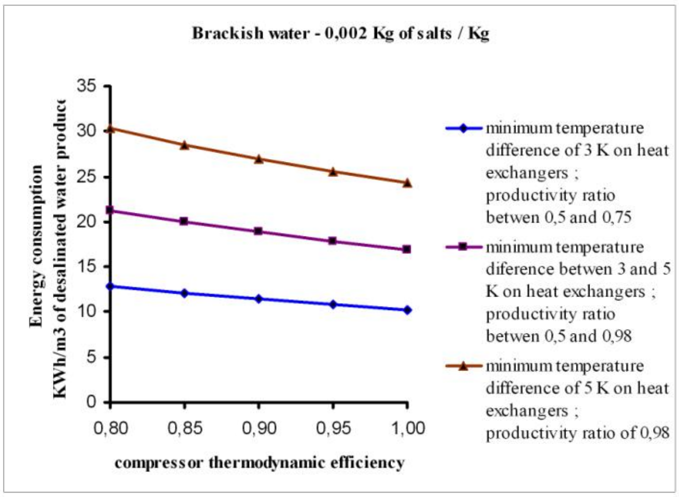


Figure 2. Energy consumption in relation to the compressor efficiency for simulations with brackish water. Concentration of 0.002 kg of salts/kg and absolute pressure in the evaporator of 121 kPa.

In the range of data in Fig. 2, the intake is between 10.26 kWh/m^3 and 30.32 kWh/m^3 of pure water produced.

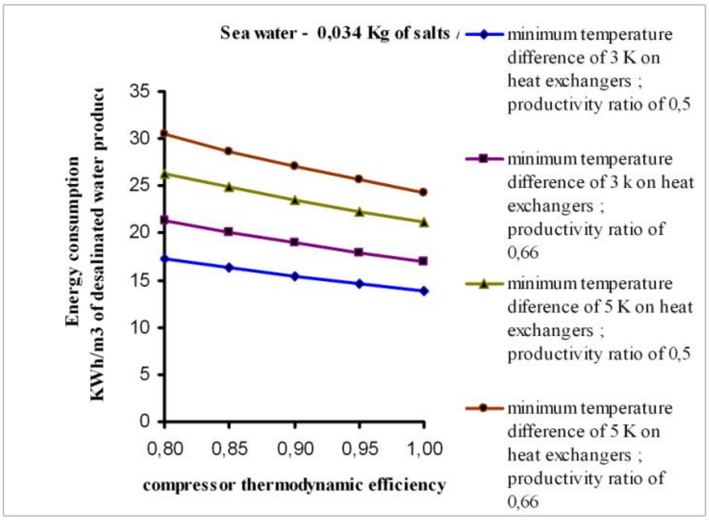


Figure 3. Energy consumption in relation to the compressor efficiency for simulations with sea water. Concentration of 0.034 kg of salts/kg and absolute pressure in the evaporator of 121 kPa.

In the range of data in Fig. 3, the intake is between 13.87 kWh/m^3 and 30.41 kWh/m^3 of pure water produced.

An increase of the flow rate of waste (reduction of productivity), and decreasing of the temperature between the fluids in the heat exchangers of the cycle, reduces power consumption.
The energy consumption in the desalination of sea water is greater due to the undesirable effect the boiling point raise proportionally to the concentration of salt solutions.

It was determined, for comparison, the amount of energy used by a single evaporator to accomplish the same proposed work without the use of any device for heat recovery. In this case the consumption rises of 10.26 kWh/m^3 p.w.p. to 808.97 kWh/m^3 p.w.p..

If the evaporation occurs at a pressure below 121 kPa, the lower pressure of the working fluid within the cycle is less than the ambient. This fact is considered undesirable because of the easy on the inlet of inert air.

The maximum temperature in the system did not exceed 160 K. The compression ratio was less than 1.7 in all cases. A low compression ratio indicates both a low power consumption in a compressor as well as a reduced consumption in the compression closed cycle with circulating fluid.

The lack of a perfect equilibrium between the amount of heat transferred and received by the heat pump, gives rise to a surplus amount of heat in the cycle, offset by the auxiliary heat exchanger. The simulations show that a fit of operating conditions turns such excess negligible.

5. CONCLUSION

We think that the technological mastery of each alternative for the production of potable water to meet the growing demand is a strategic issue for Brazil and the world. It is suggested a national research effort exploring the various alternatives available for desalination.

National efforts have been made for the purification of brackish water by reverse osmosis.

Among the advantages and disadvantages in comparison of processes by evaporation and by membranes, we have for the case of evaporation, the following points to be highlighted: (Reddy and Ghaffour, 2007 ; Ettouney and El-Dessouky, 2001; Slesarenko, 2001, Bindra and Abosh, 2001)

The durability of installation and its components is very high.
The system tends to dispense highly qualified workers
It practically exempts the chemicals consumption.
The electrical power required for the operation on the Vapor Compression Process or on Heat Pump Process may come from clean sources such as hydroelectrics, photoelectric cells or wind.
Its design, construction and constituent parts may be made or originate entirely in this country.
The proposed system does not generate thermal or chemical pollution.
The evaporation process is not subject to easy clogging or breaking of the walls.
The maintenance facilities tend to be simple.

Heat pumps, similar to conventional Vapor Compression desalination, are preliminarily indicated to service small communities. This is, however, one of many technical alternatives available for obtaining drinking water from such a source.

Globally evaporative units, desalinizing sea water, equal in capacity to those based on semi-permeable membranes.

This paper studies the obtainment of desalinated water from sea water or brackish water by employing heat pump by compression cycle. This technique may be proven effective for water purification units of small and medium sizes.

Thank you!