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Simulation of a single-stage evaporator system integrated with a mechanical vapor compressor for concentrating the electrolytic system $KNO_3 - H_2O$

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Abstract

A simulation of a single-stage evaporator system integrated with a mechanical compressor for a case study (concentrating the electrolytic system $KNO_3 - H_2O$) was performed. A mathematical model of the subsystem of a single-stage evaporator, a mechanical compressor, and superheated steam seeding is presented. Microsoft Excel with VBA (Visual Basic for Application) was used to solve the mathematical model. The model was solved by an iterative method where the values of the inlet stream temperature and the salt concentration in the concentrated stream at the evaporator outlet were assumed. The process parameters of the system have been determined. Since the goal of any industrial process is to minimize costs and maximize products, the impact of mean temperature difference changes on saturation water consumption and molar salt content in the concentrated stream was presented. 106.92 kg/h of freshwater are required to obtain 18% by weight of salt in a concentrated stream, while 432.30 kg/h of fresh water are required to obtain 25% by weight of salt in a concentrated stream. Consumption of heating steam ranged from 1760.31 to 4473.4 kg/h depending on the average temperature difference. By increasing the temperature differences from 10 to 25 °C, the amount of transferred upper lines increases from 1025 to 2750 kW, which is an advantage of increasing the mean temperature difference. The disadvantage of the larger temperature difference is the increase in the power of the mechanical compressor from 97.02 to 384.12 kW.

Keywords: Evaporation, mechanical vapor compressor, modeling, simulation, electrolyte system.

1. INTRODUCTION

Evaporation processes are the processes of removing a part of the initial rare solution and production of concentrate with different dry matter content (Ahmetović 2010). One way of concentrating salts from electrolytic systems is to use a mechanical vapor compressor integrated with a single-stage or multi-stage evaporator system. Dinnage (1975) stated that the use of a mechanical compressor can reduce energy consumption equal to the use of 30 or more evaporating degrees. Since singlestage evaporators use heating steam to concentrate salt from an aqueous salt solution, one way to reduce energy consumption is to connect the evaporator system to a mechanical or thermal steam compressor. The mechanical vapor compression can also be used in the desalination process. El-Dessouky, Alatiqi, Bingulac, and Ettouney (1998) presented a mathematical model of the multiple effect evaporation desalination process to determine the effects of the important design and operating variables on the parameters controlling the cost of producing fresh water. The mechanical vapor compressor uses secondary steam from the evaporator, which increases the pressure and temperature. Compressed steam at the outlet of a mechanical compressor is superheated steam that mixes with condensate in direct contact and is conducted into saturated steam, which is a heating medium of the

evaporation stage (Ahmetović 2010). Karić and Mustafić (2018) performed an analysis of a two-stage evaporator system and a vacuum crystallizer for the KNO₃ – H₂O electrolyte system. Karić and Mustafić (2018) showed that the amount of heat transferred in the first evaporation stage is higher than the amount of heat transferred in the second evaporation stage because the second evaporator uses secondary steam from the first evaporation stage as heating steam. Saline water refers to an aqueous solution that contains a significant concentration of dissolved salts (Ahmad & Williams 2011). Fan and Pashley (2015) presented a method for determining the enthalpy of vaporization of concentrated salt solutions using a bubble column evaporator. Ettouney, El-Dessouky, and Al-Roumi (1999) analyzed the characteristics of a singlestage evaporator with mechanical steam compression as a function of system design and operating parameters. The basic separation processes, whose synthesis and analysis can be performed using commercial process simulators, belong to distillation processes, and research related to the creation of process simulators for the separation of electrolytic systems is more recent (Suljkanović, Jotanović, Ahmetović, Tadić, & Ibrić 2013). Hong, Li, and Gu (2018) investigated the thermal performance of a mechanical vapor compression system. Hong et al. (2018) described the mathematical and experimental study of the MVC system, focusing on mathematical models that were established based on the energy and mass balance equations as well as correlations of the thermo-physical properties and heat-transfer coefficients. In this research, a mathematical model of the subsystem of a single-stage evaporator, mechanical compressor, and saturation is presented.Khanam and Mohanty (2010) developed energy reduction schemes, used to reduce the consumption of steam for a multiple-effect evaporator system. Walmsley (2016) presented a new Total Site Heat Integration method for the design of integrated evaporation systems, including vapor recompression that minimizes energy use and/or cost objective functions. The design of integrated evaporation systems is a common industrial chemical and process engineering problem (Walmsley 2016). The aim of this work is to model a single-stage evaporator with a mechanical vapor compressor and to determine the consumption of utilities.A simulation of the concentration of the KNO₃-H₂O electrolyte system was performed. The process parameters of the system have been determined. Since the goal of each industrial process is to minimize costs and maximize products, the influence of the mean temperature difference on the compressor power, saturation water consumption and molar salt content in the concentrated stream was monitored. Since each experiment at these plants is expensive, the results of this research can be used as useful guidelines for improving the work in

this process from the point of view of energy savings and increasing the amount of final product. The developed model can be applied to any two-component electrolyte system but requires the introduction of physicochemical properties of the tested electrolyte system.

2. MATERIALS AND METHODS

In the single-stage evaporator system integrated with the mechanical compressor, the electrolytic system $KNO_3 - H_2O$ is concentrated. Fresh water is introduced across the system boundaries (from the side). Flow parameters are: flow - 10000 kg/h, salt content - 0.15 wt. part. It is necessary to create an algorithm and software that determines the parameters of the process system, if the pressure in the evaporator is 0.5 bar. The size of the heating surface is 100 m², while the heat transfer coefficient is 1100 W/($m^2 \cdot K$). The average temperature difference on the heating surface of the evaporator is 10 °C, and the temperature of the water entering the saturator is 25 °C. The efficiency of the mechanical compressor is 85%. Microsoft Excel with VBA (Visual Basic for Application) was used to solve the mathematical model. The model was solved by an iterative method where the values of the inlet stream temperature and the salt concentration in the concentrated stream at the evaporator outlet were assumed.

2.1. Mathematical model

In accordance with the description of the problem above, the process scheme shown in Figure 1 was created.



Figure 1. Process scheme of a single-stage evaporator integrated with a mechanical vapor compressor.

2.1.1. Evaporation subsystem

Evaporator material balance equation:

$$\bar{m}_1 = \bar{m}_2 + \bar{m}_3$$
 (1)

Evaporator balance equation in relation to salt:

 $\bar{m}_1 \cdot$

$$c_1^{(1)} = \bar{m}_3 \cdot c_1^{(3)} \tag{2}$$

Evaporator heat balance equation:

$$\bar{m}_1 \cdot \hat{h}_1 + Q_{TR}^{(evap)} = \bar{m}_3 \cdot \hat{h}_3 + \bar{m}_2 \cdot \hat{H}_2$$
 (3)

Specific enthalpy of the inlet stream:

$$\hat{h}_1 = \int_0^{t_1} c_{p,1}(t) dt$$
 (4)

Specific heat capacity of the inlet stream (Abdulagatov, Dvoryanchikov, & Kamalov 1997):

$$c_{p,1} = f\left(c_1^{(1)}, t_1\right) \tag{5}$$

Specific enthalpy of the concentrated stream:

$$\hat{h}_{3} = \int_{0}^{t_{evap}} c_{p,3}(t) dt$$
 (6)

Specific heat capacity of the concentrated flow (Abdulagatov et al. 1997):

$$c_{p,3} = f\left(c_1^{(3)}, t_{\text{evap}}\right)$$
 (7)

Specific enthalpy of the flow of generated secondary steam (Ahmetović 2010):

$$\hat{H} = f(p_{evap}) \tag{8}$$

Secondary steam temperature (Ahmetović 2010):

$$t_s = f(p_{evap}) \tag{9}$$

Evaporator temperature:

$$t_{\text{evap}} = f\left(p_{\text{evap}}, c_1^{(3)}\right) \tag{10}$$

Transferred heat in the evaporator:

$$Q_{TR}^{(evap)} = K \cdot A \cdot \Delta t_{mean} \tag{11}$$

Mean temperature difference on the heating surface of the evaporator:

$$\Delta t_{\rm mean} = t_{hs} - t_{\rm evap} \tag{12}$$

The steam temperature at the inlet to the evaporator (Ahmetović 2010):

$$t_{hs} = f(p_{hs}) \tag{13}$$

Mass flow of heating steam:

$$\bar{m}_{hs} = \frac{Q_{TR}^{(\text{evap})}}{\Delta \hat{H}_{\nu}} \tag{14}$$

Enthalpy of condensation of heating steam (Ahmetović 2010):

$$\hat{H}_{v} = (p_{hs}) \tag{15}$$

2.1.2. Mechanical vapor compressor subsystem

Compressor energy balance equation:

$$\bar{m}_2 \cdot \hat{H}_2 + N_k = \bar{m}_2 \cdot \hat{H}_{ss} \tag{16}$$

Superheated steam:

$$\hat{H}_{ss} = \hat{H}_2 + \frac{\hat{H}_{ss}^s - \hat{H}_2}{\eta_i}$$
(17)

Specific entropy of the secondary vapor (Kozić, Bekavac, & Vasiljević 1979):

$$\hat{s} = \left(p_{\text{evap}}\right) \tag{18}$$

Specific enthalpy of superheated steam for adiabatic compression conditions (Kozić et al. 1979):

$$\widehat{H}_{ss}' = f\left(p_{hs}, \hat{s}\right) \tag{19}$$

2.1.3. Mixer subsystem

Mixer material balance equation:

$$\bar{m}_2 + \bar{m}_w = \bar{m}_{hs} \tag{20}$$

Mixer heat balance equation:

$$\bar{m}_2 \cdot \hat{H}_{ss} + \bar{m}_w \cdot \hat{h}_w = \bar{m}_{hs} \cdot \hat{H}_{hs}$$
(21)

Specific enthalpy of saturated steam (Ahmetović 2010):

$$\widehat{H}_{hs} = (p_{hs}) \tag{22}$$

Specific enthalpy of fresh water for saturation (Ahmetović 2010):

$$\hat{h}_w = f(t_w) \quad t \le 85^{\circ} \text{C}$$

$$\hat{h}_w = f(t_w) \quad t > 85^{\circ} \text{C}$$

$$(23)$$

2.2. Algorithmic steps for determining process parameters

1) The values of known parameters are entered:

$$\bar{m}_1, c_1^{(1)}, p_{\text{evap}}, A, K, \Delta t_{\text{mean}}, t_{w'} \eta_i$$

- 2) The specific enthalpy of the generated secondary vapor in the evaporator is determined \hat{H}_2 , from equation 8.
- 3) The temperature of the generated secondary steam in the evaporator t_s is determined, from equation 9.
- 4) The value of the transferred heat of the evaporator $Q_{TB}^{(evap)}$ is determined, from equation 11

- 5) The value of the specific entropy of the secondary steam *ŝ* is determined, from equation 18.
- 6) The specific enthalpy of water for saturation \hat{h}_w is determined, from equation 23.
- 7) An iterative loop for the salt content in the concentrated stream $c_1^{(3)}$ is opened, and the initial value $c_1^{(3)^{(0)}}$ is assigned to the iterative variable.
- 8) The evaporator temperature t_{evap} is determined, from equation 10.
- 9) The value of the specific heat capacity of the concentrated flow $c_{p,3}$ is determined, from equation 7.
- 10) The steam temperature at the outlet of the compressor $t_{h,s}$ is determined, from equation 12.
- 11) The specific enthalpy of the concentrated flow \hat{h}_3 is determinated, from equation 6.
- 12) The steam pressure at the outlet of the compressor p_{hs} is determined, from equation 13.
- 13) The enthalpy of condensation of heating steam $\Delta \hat{H}_{\nu}$ is determined, from equation 15.
- 14) The specific enthalpy of superheated steam \hat{H}'_{ss} is determined, from equation 19.
- 15) The specific enthalpy of saturated vapor \hat{H}_{hs} is determined, from equation 22.
- 16) The saturated steam flow \bar{m}_{hs} is determined, from equation 14.
- 17) The specific enthalpy of steam at the outlet of the compressor \hat{H}_{ss} determined, from equation 17.
- 18) The system of equations $(f_{20} \text{ and } f_{21})$ with respect to the variables $(\bar{m}_2 \text{ and } \bar{m}_w)$ is solved simultaneously.
- 19) Concentrated stream at the outlet of the evaporator m_3 is determined, from equation 1.
- 20) The compressor power N_k is determined, from equation 16.
- 21) The adjusted value for the salt content in the concentrated stream $c_1^{(3)^{(0)}}$, from equation 2.
- 22) Calculated value of the iterative variable is compared with the assumed value. If the set tolerance is reached, the accuracy of the calculation is taken to the next step. Otherwise, a new value is assigned to the iterative variable and the computer cycle is repeated by returning to algorithmic step 8

- 23) The specific enthalpy of the inlet stream \hat{h}_1 is determined, from equation 3.
- 24) An iterative loop is opened for the inlet temperature t_1 , and the iterative variable is assigned an initial value of $t_1^{(0)}$.
- 25) The value of the specific heat capacity of the inlet stream $c_{p,1}$ is determined, from equation 5.
- 26) The adjusted value for the inlet temperature $t_1^{(r)}$. is determined, from equation 4.
- 27) The calculated value of the iterative variable is compared with the assumed value. If the set tolerance is achieved, the next step is taken to calculate the accuracy. Otherwise, a new value is assigned to the iterative variable and the computer cycle is repeated by returning to the algorithmic step 24.

3. RESULTS AND DISCUSSION

The simulation results for the system of equations (1-23) are shown in Table 1. Microsoft Excel with VBA (Visual Basic for Application) was used to solve the system of equations shown in the mathematical model. The model was solved by an iterative method where the values of the inlet stream temperature and the salt concentration in the concentrated stream at the evaporator outlet were assumed. For the difference between the initial and final values of the iterative variable, a tolerance of 0.00001 was used. In contrast to the greater than the tolerance shown, a new value of the iterative variable was assumed and the procedure was repeated from the beginning. Suljkanović and Ahmetović (2008) utilized a threecomponent NaCl-KCl-H₂O system using seven variants of the evaporation-crystallization system. Suljkanović and Ahmetović (2008) determined the consumption of fuel vapor in the evaporator whose value ranged from 423.57 kg/h to 1504.35 kg/h, while the concentration of KCl ranged from 7% to 14.72% at the outlet of the evaporator, and the concentration of NaCl ranged from 15% to 25%. In this study, the consumption of heating steam ranged from 1760.31 to 4473.4 kg/h.The differences in consumption between the work of Suljkanović and Ahmetović (2008) and this research are in the use of different systems (two-component and three-component) and the fact that in this research a single-stage evaporator integrated with a mechanical steam compressor was used.

Suljkanović et al. (2013) presented a methodology for the separation of salts from three-component electrolytic systems. They created process simulators for the separation of salts from the NaCl $-Na_2SO_4-H_2O$ system for different process structures using different process

Process parameters	Mean temperature difference, °C				
	10	15	20	25	
		Stream 1			
Stream flow, kg/h	10000	10000	10000	10000	
Salt concentration, mass fraction	0.15	0.15	0.15	0.15	
Temperature, °C	84.05	79.95	75.24	69.95	
Specific enthalpy, kJ/kg	302.90	288.09	271.09	252.02	
		Stream 2			
Stream flow, kg/h	1653.44	2462.63	3261.43	4050.10	
Temperature, °C	90.4	90.57	90.80	91.10	
Pressure, bar	0.3	0.3	0.3	0.3	
Specific enthalpy, kJ/kg	2631.31	2631.31	2631.31	2631.31	
		Stream 3			
Stream flow, kg/h	8346.56	7537.37	6738.57	5949.90	
Temperature, °C	90.4	90.57	90.80	91.10	
Specific enthalpy, kJ/kg	316.09	310.58	304.08	296.32	
Fresh water stream					
Temperature, °C	25.0	25.0	25.0	25.0	
Specific enthalpy, kJ/kg	104.97	104.97	104.97	104.97	
Heating steam stream					
Stream flow, kg/h	1760.31	2653.35	3557.10	4473.40	
Temperature, °C	100.40	105.57	110.80	116.10	
Specific enthalpy, kJ/kg	2676.27	2684.94	2693.39	2701.38	
Evaporation heat, kJ/kg	2249.54	2238.68	2226.53	2213.08	
Transferred heat in the evaporator, kJ/h	3690000	5940000	7920000	9900000	
Transferred heat in the evaporator, kW	1025	1650	2200	2750	

Table 1. Simulation results for	the system of equations (1-23).
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structures that included an evaporation-crystallization system. They managed to increase the NaCl concentration from 1.3% to 9.3% in the evaporator, while they increased the Na₂SO₄ concentration in the evaporator from 2.5% to 17.88% in the acyclicstructure with water evaporation. In the structure with concentration with water evaporation and saturation with NaCl, the concentration of NaCl in the evaporator increased from 1.3% to 6.28%, while the concentration of Na₂SO₄ increased from 2.5% to 12.07% (Suljkanović et al. 2013).

In this study, the salt concentration increased from 15% to 25%. In the structure with concentration with water evaporation and saturation with NaCl, the concentration of NaCl in the evaporator increased from 1.3% to 6.28%, while the concentration of Na₂SO₄increased from 2.5% to 12.07% (Suljkanović et al. 2013). In this study, the salt concentration increased from 15% to 25%. Figures 2, 3, and 4 show the dependence of the compressor power, salt concentration in the concentrated flow, and

fresh water consumption on the mean temperature difference, respectively.

Based on Figures 2, 3, and 4, a trend of increasing compressor power, salt concentration, and fresh water consumption can be observed by increasing the average temperature difference. Increasing the mean temperature difference increases the salt concentration, but also increases water consumption and compressor power. The goal of this process is a higher concentration of salt at a minimal cost. Given that the consumption of utilities is increasing, but the salt concentration is also increasing, it is necessary to make an economic justification of this process, including the prices of the final product and utilities. Increasing the mean temperature difference from 10 to 25 °C, the amount of heat transferred increases from 1025 to 2750 kW, which is an advantage of increasing the mean temperature difference.

The disadvantage of the larger mean temperature difference is the increase in the power of the mechani-



Figure 2. Dependence of the compressor power on the mean temperature difference.



Figure 3. Dependence of the salt concentration in the concentrated flow on the mean temperature difference.

cal steam compressor from 97.02 to 384.12 kW. A higher amount of heat transfer affects the generation of a larger amount of secondary steam and higher consumption of heating steam, but there is a reduction in the flow of the concentrated stream, which results in a smaller amount of salt in the concentrated stream.

4. CONCLUSIONS

The process of salt concentration in a single-stage evaporation system with mechanical steam compression has been successfully simulated. A mathematical model of the subsystem of a single - stage evaporator, a mechanical vapor compressor, and superheated steam seeding are presented. Microsoft Excel with VBA (Visual Basic for Application) was used to solve the mathematical model. The model was solved by an iterative method where the values of the inlet stream temperature and the salt concentration in the concentrated stream at the evaporator outlet



Figure 4. Dependence of the fresh water consumption on the mean temperature difference.

were assumed. The developed mathematical model can be applied to any two-component electrolyte system but requiring the introduction of physicochemical properties of the corresponding electrolyte system. Consumption of heating steam ranged from 1760.31 to 4473.4 kg/h. The salt concentration increased from 15% to 25%. Increasing the mean temperature difference from 10 to 25 °C, the amount of heat transferred increases from 1025 to 2750 kW, which is an advantage of increasing the mean temperature difference. The disadvantage of the larger mean temperature difference is the increase in the power of the mechanical steam compressor from 97.02 to 384.12 kW, which affects the price of the mechanical compressor. Further research could go in the direction of determining the cost of increasing compressor power and increasing water consumption relative to increasing the final product.

Nomenclature

- \hat{h}_3 specific enthalpy of concentrated stream (kJ/kg)
- K heat transfer coefficient $(W/(m^2K))$
- $\bar{m_{hs}}$ flow of saturated steam at the inlet to the evaporator heating chamber (kg/h)
- $\bar{m_w}$ mass flow of water for saturation (kg/h)
- $\bar{m_1}$ inlet mass flow (kg/h)
- $\bar{m_2}$ mass flow rate of secondary vapor(kg/h)
- \bar{m}_3 mass flow of concentrated stream (kg/h)
- N_k compressor power (kW)
- *p*_{evap} evaporator pressure (bar)

- *p*_{hs} heating steam pressure (bar)
- Q_{TR} transferred heat in the evaporator (kJ/h)
- \hat{s} specific entropy of secondary steam $(kJ/(kg \cdot K))$
- t_{evap} evaporator temperature (°C)
- *t_{hs}* heating steam temperature (°C)
- *t_s* secondary vapor temperature generated in the evaporator (°C)
- t_w saturation water temperature (°C)
- t_1 temperature of the inlet stream (°C)

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