



UTILIZING VBA IN MS EXCEL FOR SIMPLIFIED SOLUTIONS IN CHEMICAL ENGINEERING: SINGLE-EFFECT EVAPORATOR STUDY

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Abstract: Solutions for an evaporator system involve equations that incorporate both mass and energy balances. Solving equations for a single-effect evaporator is simpler compared to those for multi-effect evaporator systems. However, due to the need for extensive analysis of diverse data from various sources, many prefer using simulation programs for convenience. These programs conduct calculations using their own data libraries, which contain thermodynamic and LLE-VLE data. To emulate the functionality of expensive a simulation program, an alternative interface was designed using Visual Basic for Applications (VBA) in MS Excel. In this study, we chose a single-effect evaporator system used for concentrating NaOH solution and solved its equations using a program created in VBA within MS Excel. Moreover, databases for saturated water and superheated steam data were developed within the MS Excel environment to facilitate the program. Ultimately, the program was employed to scrutinize the influence of selected parameters on other parameters, and the results were analyzed. This study serves as an illustration of how VBA in MS Excel can efficiently handle calculations pertaining to chemical engineering processes. By focusing on the single-effect evaporator, this study demonstrates how VBA in Excel can simplify and effectively conduct investigations into chemical engineering process calculations.

Keywords: Separation, Evaporation, Single-effect evaporator, Excel, Visual Basic for applications, VBA

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1. Introduction

The evaporator is a crucial device utilized across various industries, including paper, sugar, desalination, medicine, dairy, and food processing. These systems, engineered to meet specific process needs, are employed as either single-effect or multi-effect evaporators. Figure 1 illustrates a schematic representation of a single-effect evaporator.

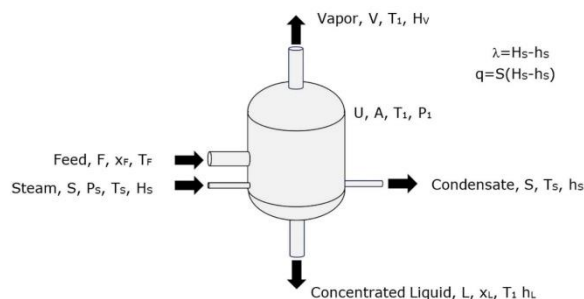


Figure 1. Scheme of an evaporator.

Various types of evaporators are utilized in different industries. An evaporator functions as a heat exchanger and is constructed from a material with a thermal conductivity coefficient, denoted as U . It is situated within a large enclosure to create a heat transfer area,

labeled A . The steam flow rate used for heating in the evaporator is represented by S . The pressure, temperature, and enthalpy values of this steam, are indicated as P_s , T_s , and H_s , respectively. This steam heats the feed flow (F), which has a concentration of x_F and a temperature of T_F . Water vapor transfers the heat load (q) to the feed, condenses, and exits the system with a saturated liquid enthalpy (h_F). Consequently, the feed reaches its boiling point (T_1), leading to the removal of the solvent in vapor form, with enthalpy H_v , from the upper part of the evaporator at a flow rate (V). This process results in a concentrated liquid stream (L), which sees an increase in concentration to x_L and possesses an enthalpy of h_L . A vacuum is applied in the vapor space at the top of the evaporator at pressure P_1 . This vacuum ensures that the product boils at lower temperatures, minimizing heat loss.

Calculations for the single-effect evaporator are divided into two parts: mass balance and heat balance calculations. The mass balance calculation starts with the feed flow rate (F), which is equal to the sum of the vapor flow rate (V) and the concentrated liquid flow rate (L) and it is written as given in Equation 1:

$$F = V + L \quad (1)$$



Total component mass balance is written as given in Equation 2:

$$F \cdot x_F = V \cdot y_V + L \cdot x_L \quad (2)$$

Since the component fraction in the vapor flow (V) in the equation $y_V=0$, it becomes Equation 3 (Çataltaş, 1963):

$$F \cdot x_F = L \cdot x_L \quad (3)$$

At this stage, the initial step involves solving Equation 3 using the available data. This culminates in the completion of the mass balance calculation through Equation 1, by employing the derived value of L. Subsequently, the heat balance calculation is initiated.

The comprehensive heat balance equation is formulated as given in Equation 4:

$$F \cdot h_F + S \cdot \lambda_S = V \cdot H_V + L \cdot h_L + Q_{lost} \quad (4)$$

In this scenario, the heat entering with the feed ($F \cdot h_F$) and the heat provided by steam heating ($S \cdot \lambda_S$) constitute the heat load in the vapor flow ($V \cdot H_V$) and the heat load in the concentrated liquid flow ($L \cdot h_L$). In this analysis, heat loss (Q_{lost}) in the system is neglected. The heat load in the exchanger is written as given in Equation 5:

$$q = U \cdot A \cdot \Delta T \quad (5)$$

Typically, the calculation of the heat exchanger area for the designed evaporator is performed using Equation 5. The calculations are then finalized by determining the steam economy using Equation 6 (Geankoplis, 1978; Geankoplis, 2003).

$$\text{Steam Economy} = V / S \quad (6)$$

In a study by Elmas (2017) in the literature, calculations for the evaporation of the NaOH solution used in the mercerization process applied to textiles were made using the approach described above. In the conducted study, in a process where the mass flow varies between 250 kg/h and 1000 kg/h, both single-effect and double-effect evaporators were used to increase the concentration of a 5% NaOH feed to 50% at a temperature of 50 °C, and the results have been analyzed. In another study, a more comprehensive but similar approach has been used to examine the optimum design and operating conditions of multi-effect evaporators used in tomato paste production. The study involves the development of a mathematical model by utilizing specific relationships for tomato concentration and a first-order degradation kinetics for lycopene. These calculations were carried out using Microsoft Excel. The findings indicate that increasing the capacity of the 5-effect evaporation system from 50 to 75 tons per hour results in an increase in lycopene yield from 95.25% to 96.27%. When examining the optimization from a total cost minimization perspective, it suggests an optimal configuration of 4 effects. However, when maximizing the Net Present Value while considering lycopene as a quality parameter, the optimal configuration is determined to be 3 effects (Simpson et al., 2008). In another study,

experimental data of the vacuum evaporation crystallization system are compared with the data obtained with the Aspen Plus simulation program. In the study at hand, both experimental and simulation results suggest that the crystallization of glycine solutions occurs at a slower rate compared to the evaporation of water. To illustrate, at a pressure of 40 mbar, while 60% of the feedwater has evaporated, only 40% of the glycine in the feed has undergone crystallization, resulting in 60% of uncrystallized glycine remaining in the feed solution. Additionally, the quantity of solid crystals produced through experimentation appears to be slightly higher than the forecasted output of the model generated by the Aspen program. According to the Aspen program model, it was anticipated that 50% of the glycine in the feed solutions would crystallize at an 80 mbar pressure, but experimental results indicate that glycine crystallized up to 60% (Said and Louhi-Kultanen, 2019).

Microsoft Visual Basic for Applications (VBA) allows users, even those without programming expertise, to record, create, and modify macros. This enables the automation of tasks within MS Office applications (Microsoft Inc., 2021).

A study highlights the significance of MS Excel in advancing Industry 4.0 in Germany. It presents four examples from chemical engineering where various programs interface with a chemical process simulator, with MS Excel playing a crucial role in most cases (Fricke and Schöneberger, 2015). The value of MS Excel and VBA in Chemical Engineering education was recognized earlier. In 2010, the Hong Kong University of Science and Technology (HKUST) began teaching Excel Visual Basic for Applications (VBA) programming in chemical engineering, focusing on enabling students to convert chemical engineering problems into functional programs (Wong and Barford, 2010). By 2016, Teppaitoon developed an Excel spreadsheet for numerical calculations in Liquid-Liquid extraction, using the 'TREND' function and mixing rule criteria for efficient problem-solving without the need for time-consuming graphing (Teppaitoon, 2016). This development underscored the need for Industry 4.0 chemical engineering students to acquire programming skills, as further emphasized in a subsequent study by Teles dos Santos, Vianna, and Le Roux (2018). Additionally, Argo et al. (2020) demonstrated an effective evaporator solution using Solid Works in conjunction with MS Excel. Similarly, Karic and Alic (2020) utilized Microsoft Excel with VBA to solve a mathematical model for integrating mechanical vapor compression into a single-effect evaporator (Karic and Alic, 2020).

Existing literature does not identify any graphical interface-based solutions for single-effect or multi-effect evaporator systems using a program. The programs developed in academic studies have evolved into paid services, continuing to support chemical and process engineering. This study aimed to solve a single-effect evaporator problem using a NaOH solution within MS

Excel, employing a graphical interface with VBA. It analyzed the effects of selected parameters on others and interpreted the results obtained.

2. Materials and Methods

A comprehensive heat and mass balance of a single-effect NaOH evaporator system has been integrated into an MS Excel program using VBA. The program's accuracy has been verified using example data from literature sources. Standard properties of water/steam and NaOH solutions have been obtained from relevant literature references.

2.1. Water/Steam Properties

The pressure, temperature, enthalpy, and heat values of water are utilized in the calculations within the evaporator system. Typically, the enthalpy and heat of vaporization are determined using pressure or temperature values. This determination often involves referencing tables or graphs of saturated and superheated water, which can require manual calculations. The data for this study, obtained from saturated water and superheated steam tables, were sourced from literature (Boles and Cengel, 2014; Geankoplis, 2003). These data were compiled into an MS Excel workbook named "Water", which is used during the evaporator calculations performed with the graphical interface.

2.2. NaOH Solution Properties

Boiling point elevation (BPE) occurs during the evaporation of NaOH solutions. The Duhring Diagram is used to determine the value of this increase. Additionally, enthalpy values are obtained using graphs that relate concentration and temperatures, which are essential in calculating the enthalpy of NaOH solutions. These data were sourced from the literature (Geankoplis, 2003; Kapuno, 2008) and compiled into an MS Excel workbook named "NaOH". The program then accesses the necessary data by referring to this workbook.

2.3. Program

The program works through a form, and a graphical interface is provided through the form. The known data on this form are given to the computer, and then the solution is reached by pressing the calculate button (Figure 2). The Calculate button activates the program related to the solution. The program was executed on a PC running MS Windows 10, equipped with 8 GB RAM and an Intel® Core™ i5-3470 CPU @ 3.20 GHz processor. During the solution process, water/steam data and NaOH solution data are calculated via interpolation in MS Excel files. These resulting data sets are then utilized in the calculation file. Additionally, at the end of the calculation, the calculated data are written into a separate file called "Report".

2.4. Single Effect NaOH Evaporator Case Study

In this case study, assuming an evaporation is used to concentrate 4536 kg/h of a 20% solution of NaOH in water entering at 60 °C to a product of 50% solid. The pressure of the saturated steam used is 172.4 kPa and the pressure in the vapor space of the evaporator is 11.7 kPa.

The thermal conductivity coefficient is 1560 W/m²·K. The requested calculation involves the steam used, the steam economy in kg vaporized/kg steam used, and the heating surface area in m² (Geankoplis, 2003). After entering the known data into the graphical interface created with VBA, the program is executed by pressing the "Calculate" button, which automatically performs the calculations. Additionally, parameters have been altered to observe their effects on the calculation. NaOH feed flowrate, NaOH feed concentration, steam pressure, vapor space pressure, thermal conductivity coefficient, concentrated liquid flow concentration, and NaOH feed temperature examined in the study. The parameters and range of values are listed in Table 1.

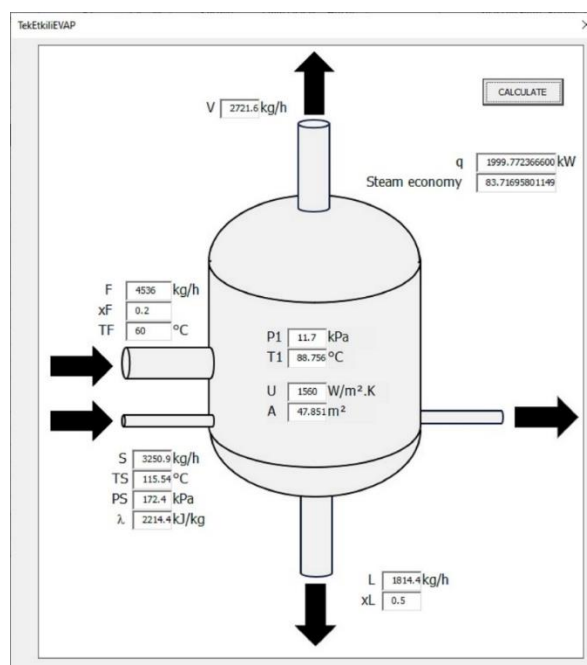


Figure 2. Graphical Interface Form in VBA workspace.

Table 1. Parameters and range of values in the study

| Parameter | Set value | Value range in the study |
|---|-----------|--------------------------|
| NaOH feed flowrate, F (kg/h) | 4536 | 1536-5536 |
| NaOH feed concentration, x_F | 0.2 | 0.01-0.49 |
| Steam pressure, P_S (kPa) | 172.2 | 75-400 |
| Vapor space pressure, P_1 (kPa) | 11.7 | 4-36 |
| Thermal conductivity coefficient, U (W/m ² ·K) | 1560 | 500-2500 |
| Concentrated liquid flow concentration, x_L | 0.5 | 0.3-0.659 |
| NaOH feed temperature, T_F (°C) | 60 | 10-100 |

3. Results and Discussion

To test programming and interface studies, a general example used in the field of Chemical Engineering was chosen. In solving this problem, the final result is the steam efficiency in the evaporator and the answer is

calculated as 83.6%. According to the example data, the calculated steam economy of the single-effect evaporator stands at 83.72% in the program. This result aligns closely with the outcome obtained using the calculation method outlined in (Geankoplis, 2003). Slight variations in the results are attributed to the precise calculation values used.

The effects resulting from changing each parameter, such as NaOH feed flow rate, F (kg/h), NaOH feed concentration, x_F , steam pressure, P_S (kPa), pressure in the vapor space, P_1 (kPa), thermal conductivity coefficient, U ($W/m^2 \cdot K$), and concentrated liquid flow concentration, x_L , are explained under separate headings below.

3.1. Effect of NaOH Feed Flowrate

The effect of the NaOH flow rate fed to the evaporator on the vapor flow rate and concentrated liquid flow rate, steam flow rate, transferred heat, and heat transfer area was investigated. During these calculations, the values of $x_F=0.2$, $T_F=60$ °C, $x_L=0.5$, $P_S=172.4$ kPa and $P_1=11.7$ kPa were kept constant, and the Feed (F) value has been changed between 1536 kg/h and 5536 kg/h.

Data illustrating the impact of the feed flow rate of NaOH on vapor flowrate, concentrated liquid flowrate, steam flowrate, transferred heat, and heat transfer area are graphically represented in Figure 3. As observed in Figure 3, an increasing trend in all these parameters is noted with the rise in NaOH feed flow rate. Furthermore, the fitted curves indicate that they all vary linearly.

3.2. Effect of NaOH Feed Concentration

The effect of the concentration of the NaOH feed to the evaporator on the vapor flow rate and concentrated liquid flow rate, enthalpy, transferred heat, heat transfer area and steam economy was examined. During these calculations, $F=4536$ kg/h, $T_F=60$ °C, $x_L=0.5$, $P_S=172.4$ kPa and $P_1=11.7$ kPa values were set and the concentration (x_F) value was changed between 0.01 and 0.49.

As a result of the calculations, the data showing the effect of the NaOH concentration fed to the evaporator on the vapor flow rate and concentrated liquid flow rate are given graphically in Figure 4. With increasing NaOH feed concentration, the vapor flow rate decreases, and the concentrated liquid flow rate increases linearly.

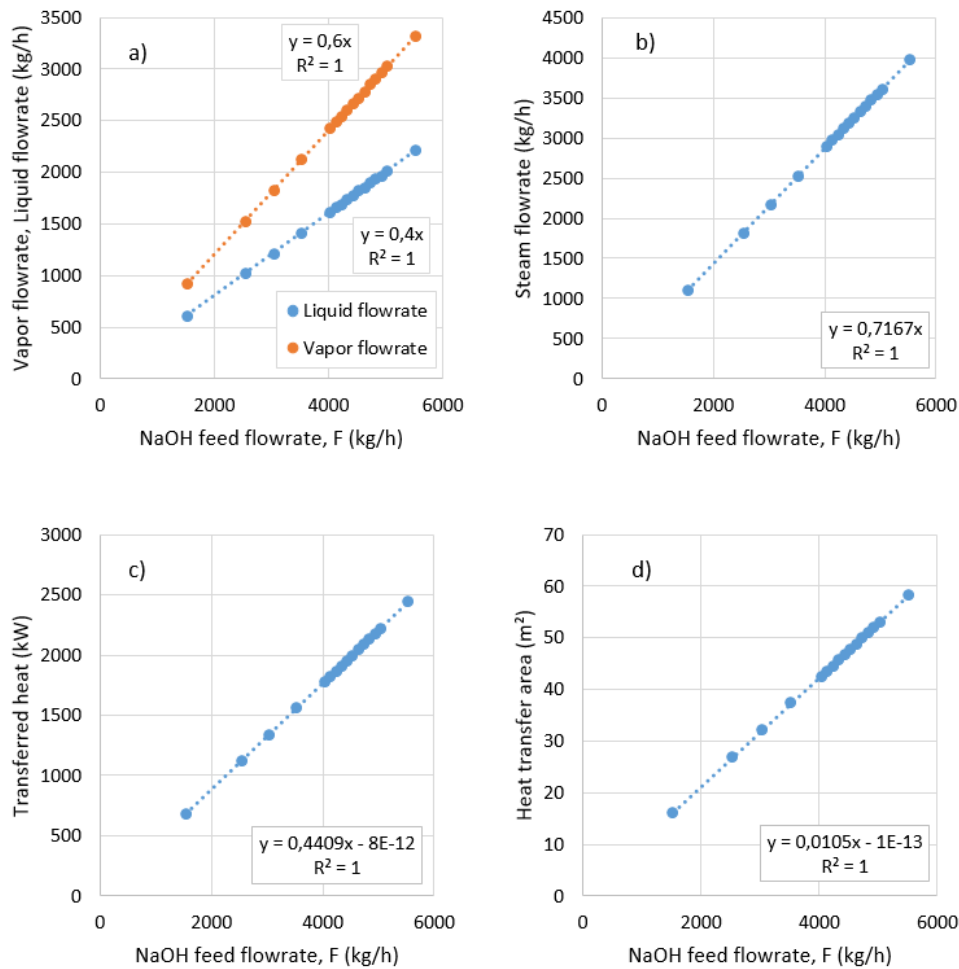


Figure 3. Effect of NaOH feed flowrate on (a) vapor and concentrated liquid flowrates, (b) steam flowrate, (c) transferred heat, and (d) heat transfer area.

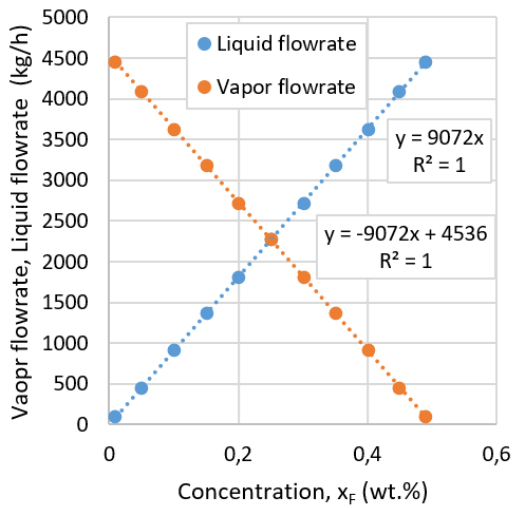
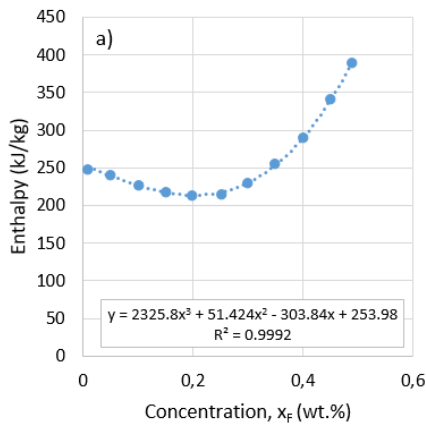


Figure 4. Effect of NaOH feed concentration on output flowrates.

In Figure 5a, data showing the effect of feed concentration on the enthalpy of the feed stream is given graphically. As a result, with increasing feed concentration, the enthalpy of the feed flow decreases first and but then it increases. The turning point is seen at $x_F=0.2$. With the curve fit, the suitability of a third-degree polynomial equation is revealed as $R^2 = 0.9992$. The increase in concentration of the NaOH feed flow causes the total transferred heat amount to decrease



(Figure 5b). It moves according to second-degree. The regression coefficient of fitted curve is 0.9999. The heat transfer area decreases with increasing feed concentration. The fitted curve is a second-degree polynomial equation with $R^2=0.9999$ (Figure 5c). The effect of feed concentration on steam economy is inversely proportional. Steam economy decreases with increasing feed concentration (Figure 5d). It has been determined that after $x_F = 0.4$, the decrease in steam economy reaches much higher values rapidly.

3.3. Effect of Steam Pressure

In the calculations made while investigating the effect of steam pressure, the values $F=4536$ kg/h, $x_F=0.2$ $T_F=60$ °C, $x_L=0.5$, and $P_1=11.7$ kPa were kept constant, and the steam pressure (P_s) value was changed between 75 kPa and 400 kPa. Figure 6a shows that the heat transfer area decreases with the increase in steam pressure. Under these conditions, the effect of using pressures higher than 125 kPa decreases on the heat transfer area. The effect of steam pressure on steam economy is appeared that steam economy decreases with increasing steam pressure (Figure 6b). It has been revealed that it can be modelled with a second-order equation, with an R^2 value of 0.9981. As the steam pressure increases, the steam flowrate increases. By the modelling for the data, the fitted curve fits a second order function and the R^2 is 0.9986 (Figure 6c).

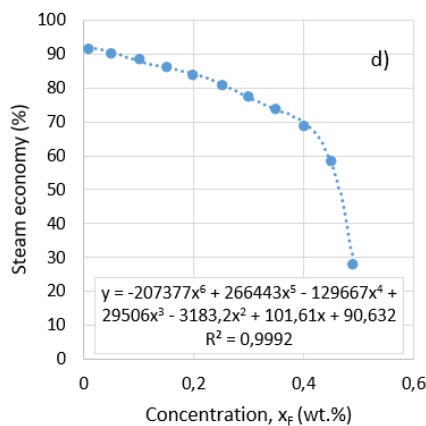
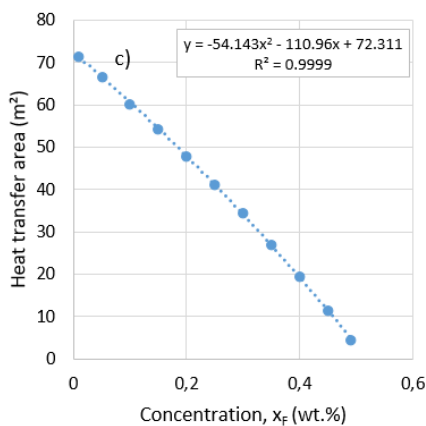
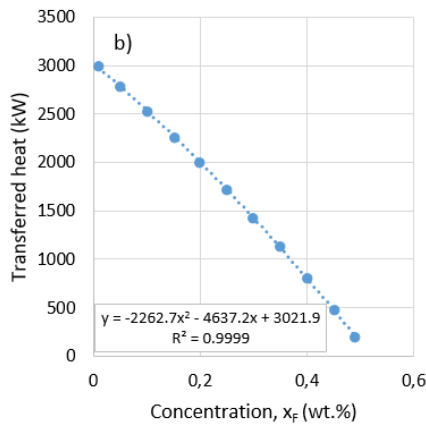


Figure 5. Effect of NaOH feed concentration on (a) enthalpy of concentrated liquid flow, (b) transferred heat, (c) heat transfer area, and (d) steam economy.

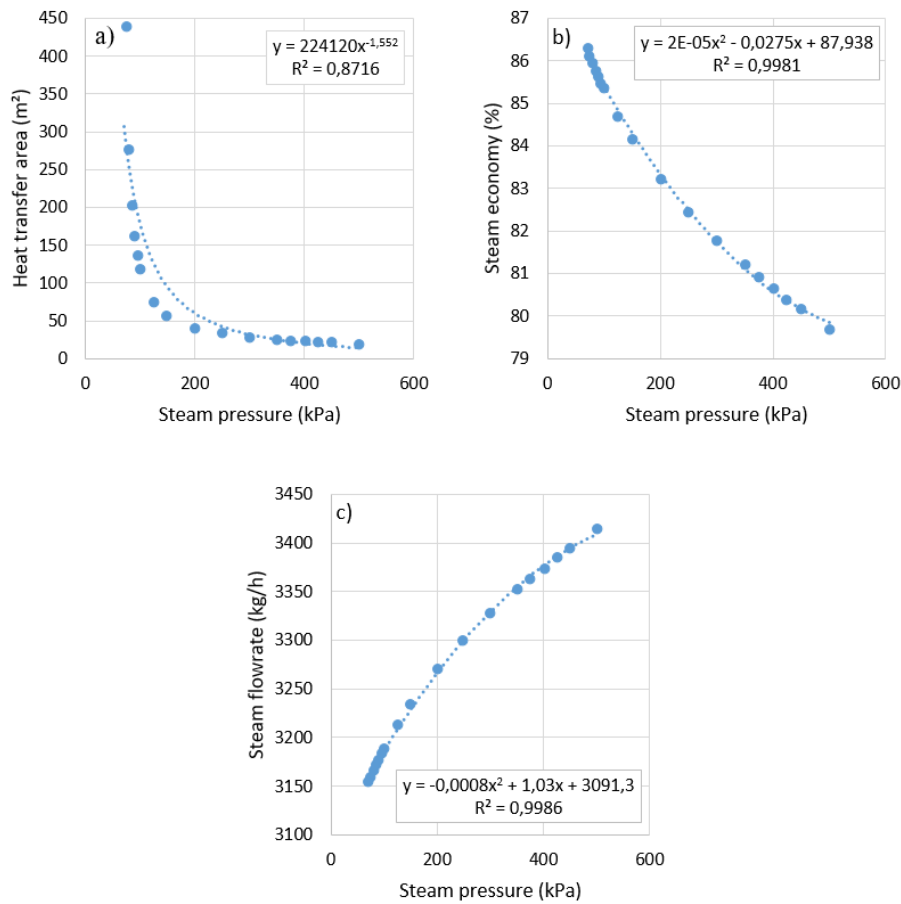


Figure 6. Effect of steam pressure on (a) heat transfer area, (b) steam economy, and (c) steam flowrate.

3.4. Effect of Pressure in the Vapor Space

In the series of calculations examining the effect of the pressure in the vapor space of the evaporator, the values $F=4536$ kg/h, $x_F=0.2$ $T_F=60$ °C, $x_L=0.5$, and $P_S=172.4$ kPa were kept constant, and the pressure (P_1) value increased from 4 kPa to 36 kPa (Figure 7).

It can be seen in Figure 7a that increasing the pressure in the vapor space of the evaporator causes the boiling point elevation to increase. When these data are modelled, an exponential function with an R^2 value of 0.9971 is obtained. The increase in vapor space pressure leads to an increase in the transferred heat. Additionally, the model suggested for the total transferred heat can be represented by an exponential function. The R^2 value of the function is 0.9979 (Figure 7b). Figure 7c shows that the heat transfer area increases with the increase in pressure in the vapor space of evaporator. After the pressure reaches 30 kPa, the increase in the heat transfer area accelerates. Another parameter examined is the variation in steam economy. As the pressure in the vapor space increases, steam economy decreases. It is observed that it can be modeled with a logarithmic function, where the R^2 value is obtained as 0.9990. The impact of pressure in the evaporator's vapor space on steam economy is presented in Figure 7d.

3.5. Effect of Thermal Conductivity Coefficient

While making calculations examining the effect of the thermal conductivity coefficient, U on the heat transfer

area, A , the values of $F=4536$ kg/h, $x_F=0.2$ $T_F=60$ °C, $x_L=0.5$, $P_S=172.4$ kPa and $P_1=11.7$ kPa are constant was kept, the coefficient (U) value was changed between 500 $W/m^2 \cdot K$ and 2500 $W/m^2 \cdot K$. The calculations in the study determine that with the increase in the thermal conductivity coefficient, the heat transfer area in the evaporator is exponentially related and decreases (Figure 8).

3.6. Effect of Concentrated Liquid Flow Concentration

In the calculations made while examining the effect of concentrated liquid flow concentration on heat transfer area, concentrated liquid flow rate, steam economy and steam flow rate, $F=4536$ kg/h, $x_F=0.2$ $T_F=60$ °C, $P_S=172.4$ kPa and $P_1=11.7$ kPa values were kept constant, and the x_L parameter was changed between 0.3 and 0.659. Increasing the concentrated liquid flow concentration causes the heat transfer area in the evaporator to increase (Figure 9a). Although the concentration (x_L) parameter shows an almost linear trend up to 0.5, this linearity breaks down after 0.6 and the heat transfer area increases more rapidly. With the increase in concentration of the concentrated liquid flow, the concentrated liquid flow rate and steam economy exhibit a decrease (Figure 9b and Figure 9c), in contrast, the vapor flow rate is observed to increase (Figure 9d). The behavior of these parameters aligns with second-order models.

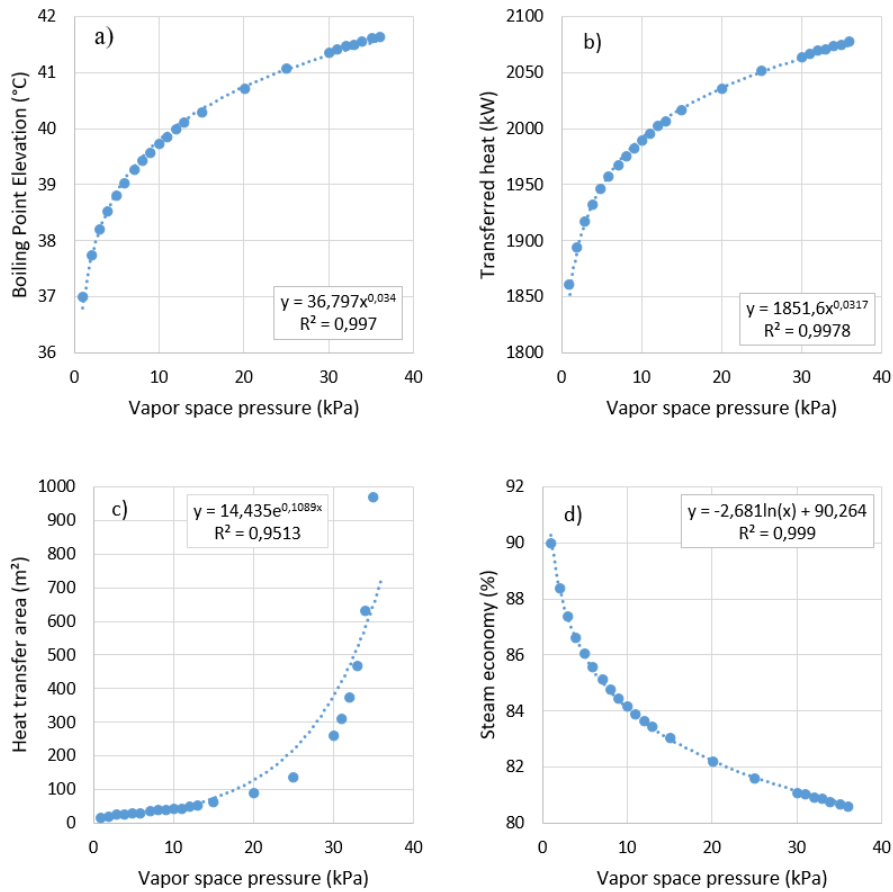


Figure 7. Effect of vapor space pressure on (a) BPE, (b) transferred heat, (c) heat transfer area, and (d) steam economy.

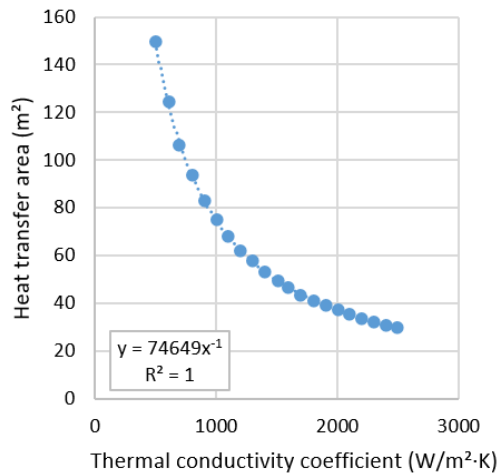


Figure 8. Effect of thermal conductivity coefficient on heat transfer area.

3.7. Effect of NaOH Feed Temperature

NaOH feed temperature changing affects the feed temperature, enthalpy, total transferred heat, heat transfer area, steam economy and work steam flow rate. During the calculations, the values of $F=4536$ kg/h, $x_F=0.2$, $x_L=0.5$, $P_S=172.4$ kPa and $P_I=11.7$ kPa were kept constant, and the temperature (T_F) parameter was changed between 10 °C and 100 °C. As the temperature increases, all parameters examined in the evaporator behave linearly. For all other parameters besides steam economy, the regression coefficient is found to be 1

($R^2=1$). Figure 10 displays the models with which they are compatible. As illustrated in the figure, with an increase in feed temperature, enthalpy and steam economy increase, while the transferred heat, heat transfer area, and steam flow rate decrease.

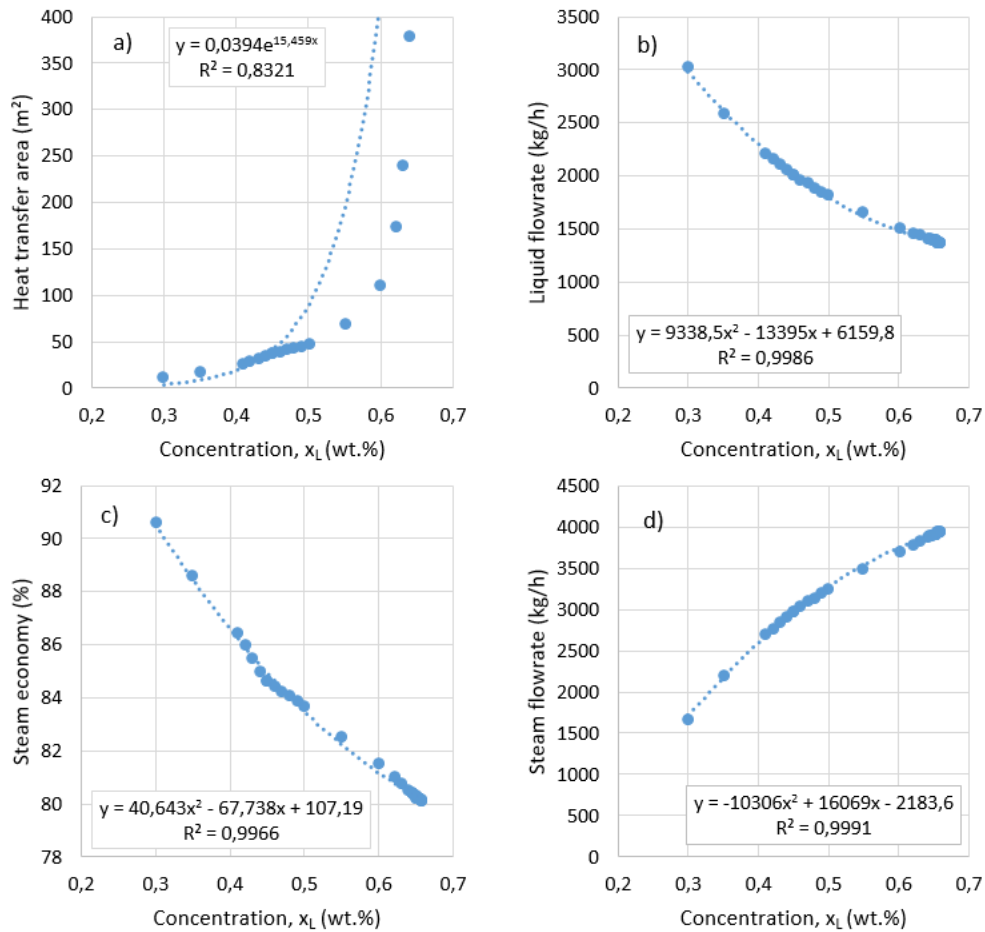


Figure 9. Effect of concentrated liquid flow concentration on (a) heat transfer area, (b) concentrated liquid flowrate, (c) steam economy, and (d) steam flowrate.

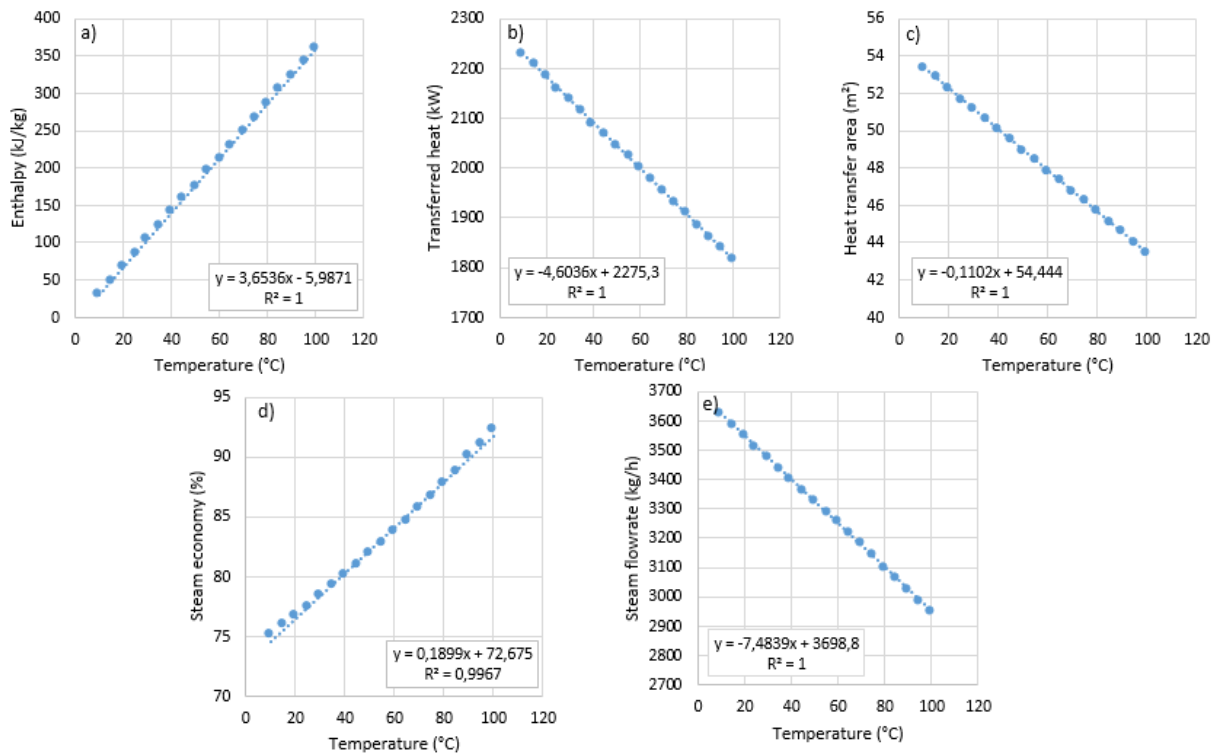


Figure 10. Effect of feed temperature on (a) enthalpy of concentrated liquid flow, (b) transferred heat, (c) heat transfer area, (d) steam economy, and (e) steam flowrate.

4. Conclusion

The most important result of the study is the ease of performing calculations for a single-effect evaporator using the graphical interface designed with VBA in the MS Excel program. This has enabled the calculation of missing data for NaOH solutions in a single-effect evaporator using known values, through the designed interface and the written program. Thanks to flexible programming, it is also possible to arrange designs for new solutions. Additionally, the effects of changing certain parameters on others were investigated using the calculations performed by the program, and the results are summarized below:

- The NaOH feed flow rate is directly proportional to the vapor flow rate, concentrated liquid flow rate, steam flow rate, total transferred heat, and heat transfer area.
- The NaOH feed concentration is inversely proportional to the vapor flow rate and directly proportional to the concentrated liquid flow rate.
- As the NaOH feed concentration increases, the feed enthalpy first decreases and then increases after reaching its lowest value of 0.2. This situation stems from enthalpy-concentration-temperature data in the literature.
- The NaOH feed concentration is inversely proportional to the total transferred heat, heat transfer area, and steam economy, and the steam economy drops rapidly after the value of 0.45.
- The steam pressure is directly proportional to the steam flow rate and inversely proportional to the heat transfer area and steam economy. It has been determined that the heat transfer area increases significantly, especially when the pressure is lower than 74.72 kPa.
- With the increase in pressure in the vapor space, the boiling point elevation, total transferred heat, and heat transfer area increase, especially after 25 kPa, the heat transfer area increases rapidly. The steam economy decreases with the increase in pressure.
- As expected, a relationship is given for the decrease in the heat transfer area with the increase in the thermal conductivity coefficient.
- With the increase in the concentration of the concentrated liquid flow, a decreasing effect is observed on the concentrated liquid flow rate and steam economy, while an increasing effect is seen on the heat transfer area and steam flow rate. Especially after the concentrated liquid concentration reaches 0.55, the heat transfer area increases rapidly.
- The feed flow temperature is directly proportional to the feed flow enthalpy and steam economy, and inversely proportional to the total transferred heat and heat transfer area.

Author Contributions

The percentage of the author contributions is presented below. The author reviewed and approved the final version of the manuscript.

| | M.B.A. |
|-----|--------|
| C | 100 |
| D | 100 |
| S | 100 |
| DCP | 100 |
| DAI | 100 |
| L | 100 |
| W | 100 |
| CR | 100 |
| SR | 100 |
| PM | 100 |
| FA | 100 |

C=Concept, D= design, S= supervision, DCP= data collection and/or processing, DAI= data analysis and/or interpretation, L= literature search, W= writing, CR= critical review, SR= submission and revision, PM= project management, FA= funding acquisition.

Conflict of Interest

The author declared that there is no conflict of interest.

Ethical Consideration

Ethics committee approval was not required for this study because of there was no study on animals or humans.

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