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Original Article

Artificial Water Hardness Removal-Modelling and Simulation in ASPEN Plus

Isa Umaru Usman[1], Abdulhalim Musa Abubakar[2], Bukar Ibrahim Askira[3], Moses NyoTonglo Arowo[4], Abba Saleh Lawan[5], Tahiru Saka[6]

[1,2,3,5,6]*Department of Chemical Engineering, Faculty of Engineering, University of Maiduguri (UNIMAID), Bama Road Maiduguri, Borno State, Nigeria.*
[2]*Department of Chemical Engineering, Faculty of Engineering, Modibbo Adama University (MAU), Yola, Adamawa State, Nigeria.*
[4]*Department of Chemical & Process Engineering, Moi University, Eldoret, Kenya.*

[2]abdulhalim@mau.edu.ng

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Abstract - ASPEN Plus is not often a satisfactory software for modelling and simulation of water treatment plants, as it lacks the support for the presence of microorganisms, large debris, leather and other impurities. However, the study herein shows that the software can simulate a simple hard water softening plant, a phenomenon that is important for home and industrial use. Three m^3 of artificial hard water containing 288 kg $CaCl_2$, 390 kg $NaHCO_3$, and 220 kg of $MgSO_4.7H_2O$ was softened by passing it through different units defined using ASPEN Plus V8.8. The initial mole percent of the hardness chemicals added was 12.84 %, resulting in soft water containing trace amounts of all the hardness chemicals. Separation of the minerals from the hard water was achieved using an evaporator unit 'Flash2', where the temperature above the boiling point of the compound or mineral salt with the highest boiling point was specified. Almost 100% soft water was achieved when the simulation converged. This work, therefore, addresses the potential negative effects associated with the use of hard water by humans and animals. Engineering such a scheme for implementation across all water treatment facilities would be a welcoming idea, as it will help reduce the challenges faced by end-users of clean hard water supply.

Keywords - Distilled water, Hard water, Tap water, Water treatment, Soft water.

1. Introduction

Hard water is water containing chlorides, sulphides and bicarbonates of calcium and magnesium [1, 2]. Water hardness is classified into permanent and temporary hardness [3]. Temporary hardness can be eliminated by the simple act of boiling the water. The constituents of temporary and permanent hard water varies. The hardness of water is defined in terms of mg $CaCO_3$/L or mg Calcium/L. Both water hardness types are still considered drinkable if they house the right amount of mineral elements. Water treatment scientists must, therefore, ensure that treated water from water treatment plants is tested for various quality parameters. Quality water can be described as odourless, colourless, tasteless and having the correct proportion of other chemicals [4]. In the literature, standards or threshold limits of water constituents are well defined [5–7].

Key benefits of utilizing soft water include the prevention of limescale buildup in pipes, appliances and fixtures, minimization of soap scum and residue formation in dishes and glassware, enhancement of softer and smoother skin and hair, improvement of soap and detergent efficiency, increment in water efficiency, energy savings in water heaters, taste and clarity upgrading and clothes life span increment.

It is, therefore, necessary to remove/reduce water hardness prior to use. The use of ASPEN Plus for water softening, especially general wastewater treatment, is constrained by several factors, hence limiting its application. One such major limiting factor is the inability or difficulty in utilizing the software to model several water separation and treatment processes [8]. This study, therefore, aims to create an artificial hard water based on an existing hard water constituent's composition found in the literature and to use the artificial hard water as feed to an ASPEN Plus modelled and simulated water softening plant. The methodology consists of the appropriate feed stream, unit selection and specifications, following a simple chemical process NRTL thermodynamic property model. Also, a simple distillation or evaporation process, as described in the literature [9–12], is incorporated into the design.

2. Materials and Method

2.1. ASPEN Plus Component Specification

Advanced System for Process Engineering (ASPEN) Plus V8.8 was used to define an artificial hard water constituents using the NRTL thermodynamic property model, as shown in Figure 1.

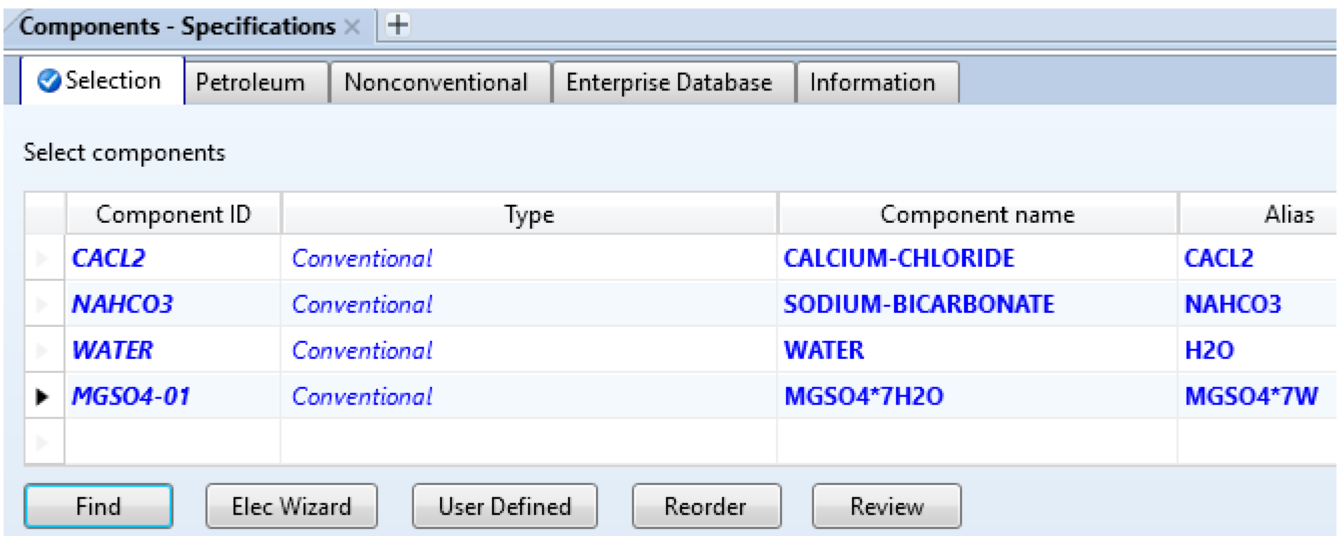


Fig. 1 Components entry for the mock hard water model

All species selected were conventional compounds with known or specific structures and chemical formulas. They include Calcium Chloride ($CaCl_2$), Sodium Bicarbonate ($NaHCO_3$), pure Water (H_2O) and Magnesium Sulphate Heptahydrate ($MgSO_4.7H_2O$). The boiling points and forms of the compounds in Figure 1, as shown in Table 1, were used to define all process inputs during ASPEN Plus simulation conveniently.

Table 1. Boiling points and appearance of species used

S/No.	Chemical Formulae/Component	Molecular Weight (kg/mol)	Boiling Point (°C)	Phase
1.	H_2O	18.01528	100	Liquid
2.	$NaHCO_3$	84.007	851	White solid
3.	$CaCl_2$	110.98	1935	Solid white
4.	$MgSO_4.7H_2O$	246.48	330	Solid

All inputs in the simulation were defined as liquid to eliminate the need for additional units for slurring them before feeding into the main system since they are also present in liquid form. Hence, a solution of $NaHCO_3$, $CaCl_2$ and $MgSO_4.7H_2O$ was defined.

2.2. Feed Stream and Block Specification

A separate stream of tap water (TAP-H_2O), which is very clean water, was mixed with another stream of hard water chemicals (H-CHEM1) by charging them to a tank (MIX-TANK). Their flow conditions and amounts were defined in ASPEN Plus, as shown in Figures 2 and 3.

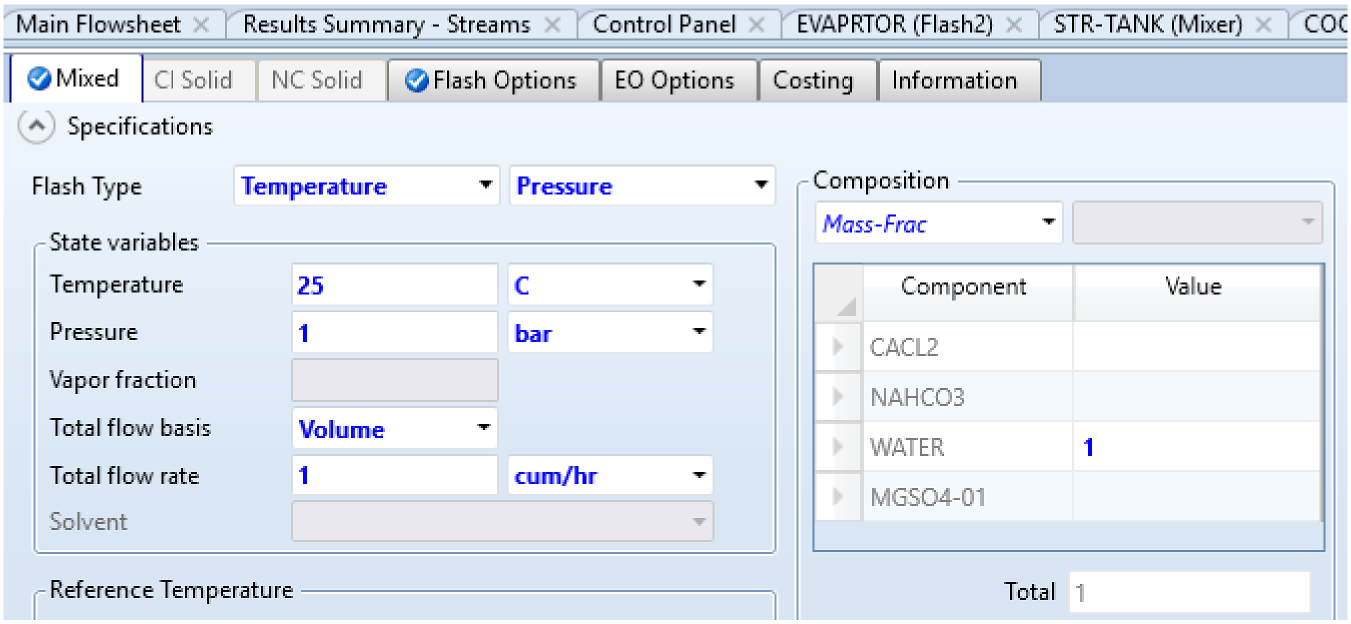


Fig. 2 Pure tap water temperature and pressure conditions

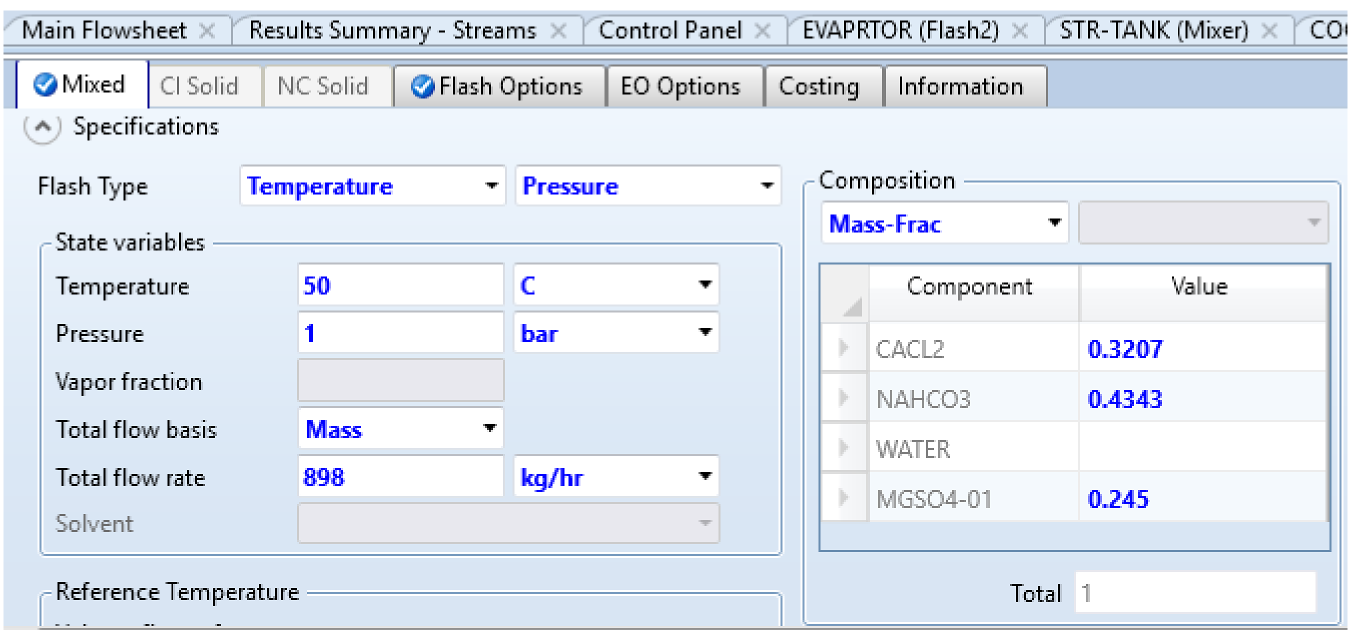


Fig. 3 Hard water chemical stream weight percent

Figures 2 and 3 show that hard water stream specification was defined in accordance with the definition found in Hettiarachchi et al. (2017), where 1 dm^3 of distilled water containing 288 mg $CaCl_2$, 220 mg $MgSO_4.7H_2O$ and 390 mg $NaHCO_3$ was created artificially. In this work, the amount fed was scaled up and specified in SI units in ASPEN Plus.

From ASPEN Plus 'Model Palette', 5 blocks were defined, including 2 tanks, 2 heat exchangers and 1 separator, as shown in Table 2.

Table 2. Block specification

S/No.	Block	Operating Condition	Valid Phase
1.	Mix-Tank	0 bar	Liquid-Only
2.	Heater	70°C & 1 atm	Vapor-Liquid
3.	Evaporator	2000°C & 1 atm	Vapor-Liquid
4.	Cooler	25°C & 1 atm	Liquid-Only
5.	STR-Tank	0 bar	Liquid-Only

Valid phases of the respective units were defined accordingly by following the process description. After completing all input specifications, the ASPEN Plus simulation was run to test for convergence.

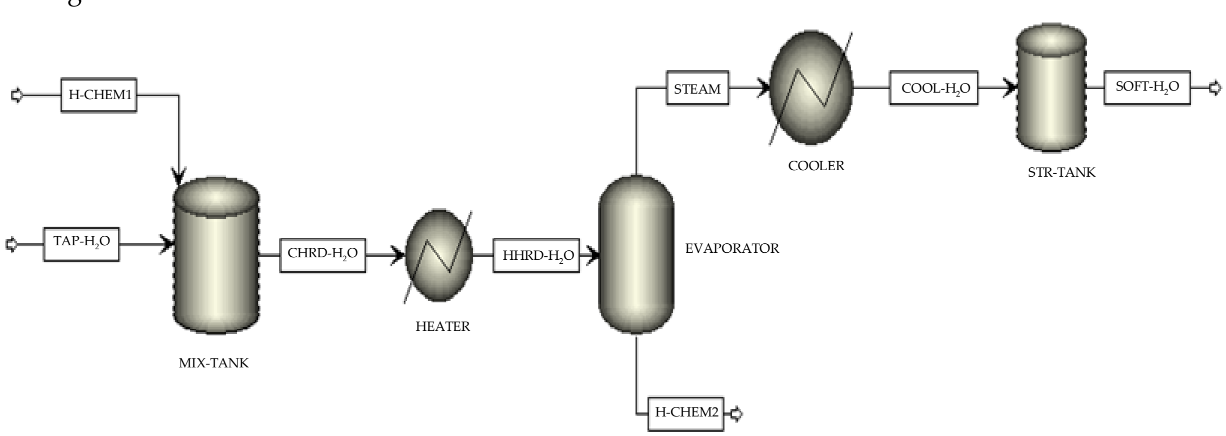
2.3. Process Description

TAP-H_2O stream containing 1 m^3 of clean water at 25°C and 1 atm was fed to a tank (MIX-TANK). Another stream containing $CaCl_2$ (32.07 wt%), $NaHCO_3$ (43.43 wt%) and $MgSO_4.7H_2O$ (24.5 wt%) was fed through H-CHEM1 stream to the same tank to facilitate mixing in order to create an artificial hard water (at 50°C). 'H-CHEM1' stands for hardness chemical feed stream 1. The exit mixture or cool hard water stream (CHRD-H_2O) from MIX-TANK was heated to 70°C using a Heater. The hot hard water stream (HHRD-H_2O) from the HEATER was routed to a separator 'Flash2' (tagged Evaporator) to model a simple evaporation process. Based on the boiling temperatures of the hardness chemicals given in Table 1, the Evaporator was kept at 2000°C to cover the entire boiling points of fluid coming to the block. Hot water, as steam or vapor, was ejected through the STEAM stream while the liquid stream containing hardness chemicals was exited via the H-CHEM2 stream of the Evaporator. In order to cool the distilled water stream (i.e., STEAM stream), it was sent to a Cooler operating at 25°C. COOL-H_2O stream was produced and stored as SOFT-H_2O (soft water) in STR-TANK or storage tank.

3. Results and Discussion

3.1. Process Flow Diagram

Following the process described in the methodology, the overall process flow diagram was generated, as shown in Figure 4.



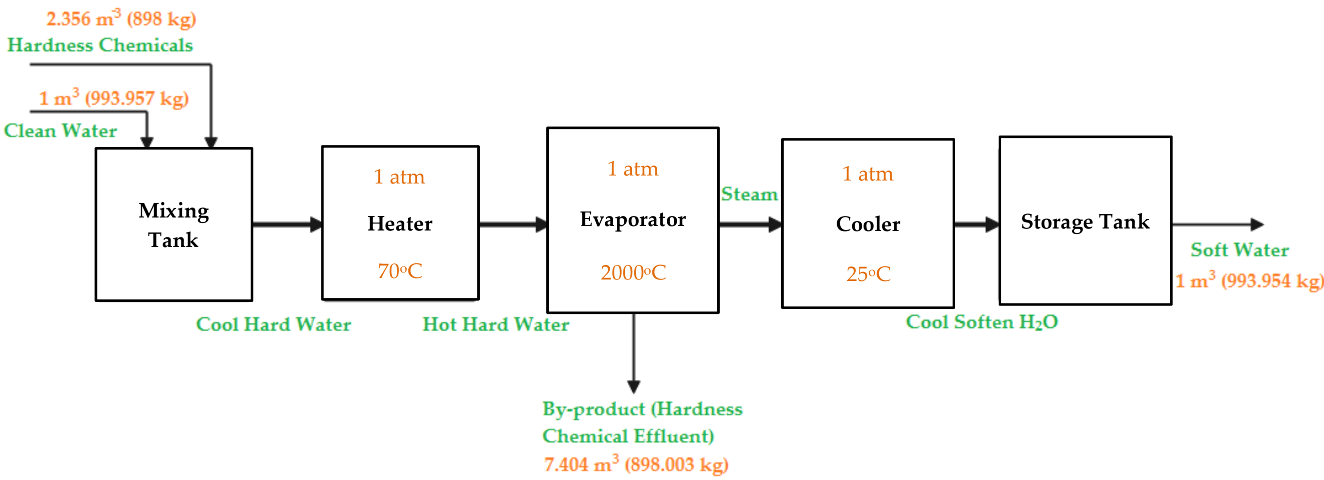


Fig. 4 Water softening plant process and block flow diagram

Figure 4 shows a systematic arrangement or configuration of units to enable soft water production based on their mode of operation and characteristics as defined by ASPEN Plus.

3.2. Stream Results

Table 3 shows the stream results of the entire process, as illustrated in Figure 4.

Table 3. ASPEN plus simulation outcome

	H-CHEM1	TAP-H_2O	CHRD-H_2O	HHRD-H_2O	STEAM	H-CHEM2	COOL-H_2O	SOFT-H_2O
Temperature (°C)	50	25	28.4	70	2000	2000	25	25
Pressure (bar)	1	1	1	1.013	1.013	1.013	1.013	1.013
Vapor Frac	0	0	0	0	1	0	0	0
Mole Flow (kmol/h)	8.13	55.173	63.303	63.303	55.173	8.13	55.173	55.173
Mass Flow (kg/h)	898	993.957	1891.957	1891.957	993.954	898.003	993.954	993.954
Volume Flow (m^3/h)	2.356	1	3.079	3.131	10291.15	7.404	1	1
Enthalpy (Gcal/h)	-0.473	-3.766	-4.239	-4.191	-2.04	-0.172	-3.766	-3.766
CACL2	2.595		2.595	2.595	trace	2.595	trace	trace
NAHCO3	4.642		4.642	4.642	trace	4.642	trace	trace
WATER		55.173	55.173	55.173	55.173	< 0.001	55.173	55.173
MGSO4-01	0.893		0.893	0.893	trace	0.893	trace	trace

It is important to keep water at room temperature to allow its use for drinking, industrial cooling applications and other domestic uses, as illustrated in Table 3. Additionally, heat duties of HEATER, COOLER and EVAPORATOR blocks are presented in Appendix A.

3.3. Discussion

The artificial water hardness removal process was modeled and simulated using the ASPEN Plus NRTL property model. An almost equal amount of the hardness chemicals fed was discharged as a by-product via H-CHEM2 stream containing < 0.001 kmol/h of water. The process resembles a simple distillation apparatus in the laboratory for distilled water production. Although there are still some trace amounts of the hardness chemicals in the soft water produced, the amounts are less than those reported in the literature for soft water [14]. Precisely, 3.079 m^3/h of hard water (CHRD-H_2O) gives 1 m^3 of soft water, indicating that almost the entirety of the volume of the tap water fed was produced. A temperature of 2000°C specified in the evaporator was sufficient to melt the hard chemicals and hence facilitate their flow as a liquid via the H-CHEM2 stream.

4. Conclusion

The study herein shows the possibility of constructing a water-softening plant to practically reduce/remove water hardness from tap water to enhance its quality further. The ASPEN Plus design utilizes approximately 3 m^3 of an existing artificially created hard water in the literature to feed a water-softening plant model. Results show that the resulting water is 99.99+ % soft. Furthermore, no additional chemical is fed into the process. The cost associated with constructing a water-softening plant is necessary to implement a successful hard water transformation process to create an eco-friendly environment.

Data Availability

All data, as displayed in the Tables and Figures shown in this work, are the entire results obtained during the research. Thus, the ASPEN Plus simulation file is available and may be delivered upon request after satisfying personal terms, which will be made known by the corresponding author. Emails requesting the ASPEN Plus file on this study should be directed to abdulhalim@mau.edu.ng.

Authors' Contributions

The conceptualization of the work is attributed to A.M.A. Methodology, as described by B.I.A. At the same time, software utilization and result validation were carried out by I. U. U. Most importantly, A.S.L., A.M.A., and M.N.A. collectively carried out the formal Analysis, investigation, resource search, and data curation. Writing–original draft preparation as well as writing–review & editing was done by A.M.A and B.I.A. Visualization, supervision, and project administration are credited to M.N.A. Funding acquisition was facilitated by T.S.

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References

[1] D.V.S.S. Ramavataram, "Drinking water-Hard or soft?," *National Journal of Community Medicine*, vol. 3, no. 1, pp. 1–2, 2012. [Google Scholar] [Publisher Link]

[2] Pallav Sengupta, "Potential Health Impacts of Hard Water," *International Journal of Preventive Medicine*, vol. 4, no. 8, pp. 866–875, 2013. [Google Scholar] [Publisher Link]

[3] T. Ganesh et al., "Experiments for Calculating Properties of Distilled Water from Solar Still and Potable Water from Reverse Osmosis Process," *International Journal of Recent Technology and Engineering*, vol. 8, no. 4, pp. 1780–1785, 2019. [CrossRef] [Publisher Link]

[4] Abdulhalim Musa Abubakar et al., "Water Treatment Operations: Case Study of Mada Water Works," *Water Treatment Operations: Case Study of Mada Water Works*, vol. 9, no. 3, pp. 21–37, 2022. [CrossRef] [Google Scholar] [Publisher Link]

[5] WHO, *Guidelines for Drinking-Water Quality: Incorporating the First Addendum*, 4th ed., Geneva: World Health Organization (WHO), 2022. [Google Scholar] [Publisher Link]

[6] Miklas Scholz, *Wetland for Water Pollution Control*, 2nd ed., Elsevier, pp. 1–5, 2016. [Google Scholar] [Publisher Link]

[7] Yirdaw Meride, and Bamlaku Ayenew, "Drinking Water Quality Assessment and its Effects on Residents Health in Wondo Genet Campus, Ethiopia," *Environmental Systems Research*, vol. 5, no. 1, pp. 1–7, 2016. [CrossRef] [Google Scholar] [Publisher Link]

[8] Francis B. Elehinafe et al., "Insights on the Advanced Separation Processes in Water Pollution Analyses and Wastewater Treatment-A Review," *South African Journal of Chemical Engineering*, vol. 42, pp. 188–200, 2022. [CrossRef] [Google Scholar] [Publisher Link]

[9] T. Z. Farge, K. F. Sultan, and A. M. Ahmed, "Experimental Study of the Performance Water Distillation Device by using Solar Energy," *Engineering and Technology Journal*, vol. 35, no. 6, pp. 653–659, 2017. [CrossRef] [Google Scholar] [Publisher Link]

[10] Habila Adamu et al., "Development of a Solar Water Distiller and Laboratory Analysis of the Product," *ABUAD Journal Engineering Research Development*, vol. 1, no. 2, pp. 211–217, 2018. [Google Scholar] [Publisher Link]

[11] M.A. Hassan et al., "Development of a Laboratory-Scale Solar Water Distiller," *International Journal of Scientific Research in Science, Engineering and Technology*, vol. 3, no. 5, pp. 39–46, 2017.[Google Scholar] [Publisher Link]

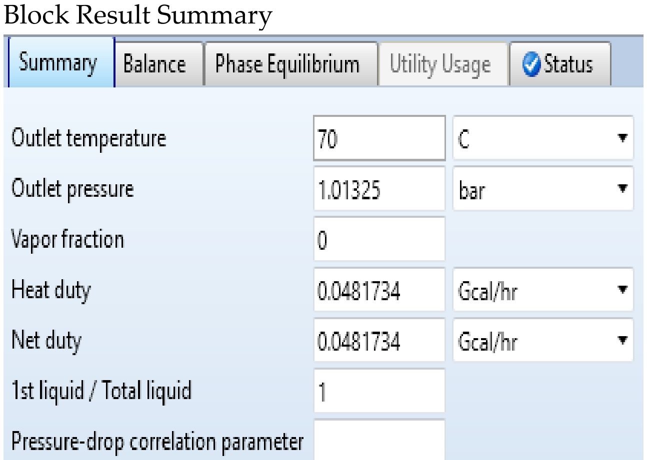
[12] Naseer T. Alwan, S. E. Shcheklein, and Obed M. Ali, "Evaluation of Distilled Water Quality and Production Costs from a Modified Solar still Integrated with an Outdoor Solar Water Heater," *Case Studies in Thermal Engineering*, vol. 27, 2021. [CrossRef] [Google Scholar] [Publisher Link]

[13] Eshani Hettiarachchi, Nilwala Kottegodab, and A. D. L. Chandani Perera, "Activated Coconut Coir for Removal of Water Hardness," *Desalination and Water Treatment*, vol. 66, pp. 103–110, 2017. [CrossRef] [Google Scholar] [Publisher Link]

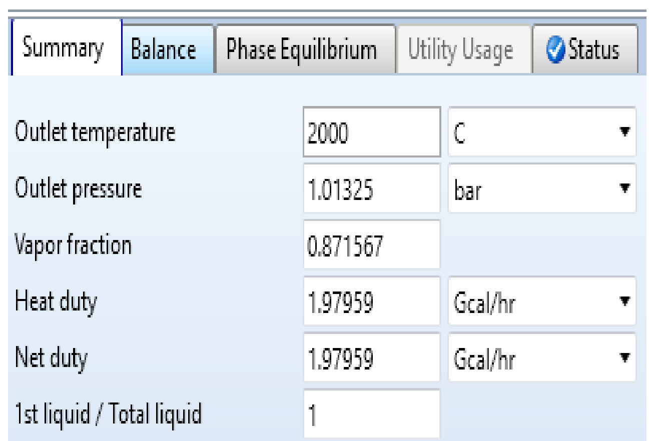
[14] Min Kyung Ahn et al., "Removal of Hardness from Water Samples by a Carbonation Process with a Closed Pressure Reactor," *Water*, vol. 10, no. 1, pp. 1-10, 2018. [CrossRef] [Google Scholar] [Publisher Link]

Appendix A

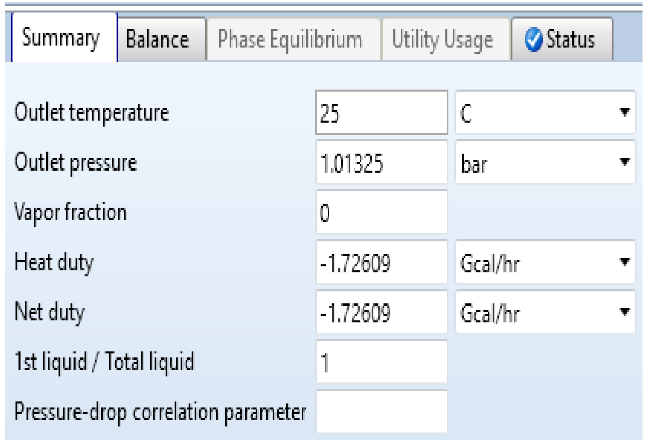
Block Result Summary



(a) Evaporator



(b) Heater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bar
Vapor fraction
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Gcal/hr
Net duty
-1.72609
Gcal/hr
1st liquid / Total liquid
1
Pressure-drop correlation parameter
(c) Cooler