

# Simulation-Assisted Evaluation of Salt Purification for Industrial Textile Applications

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**Abstract**— *The textile industry requires high-purity salt as a critical raw material for dyeing. However, in many developing countries, including Honduras, locally produced marine salt does not consistently meet industrial purity specifications, resulting in dependency on imports and higher production costs. This study presents the design, and simulation of a marine salt purification process aimed at textile-grade applications, using Aspen Plus as the primary modeling tool. The proposed process integrates brine pretreatment, chemical coagulation, filtration, heat exchange, vacuum crystallization, centrifugation, and convective drying. An electrolyte-based thermodynamic model was implemented to accurately represent salt dissociation, impurity precipitation and phase behavior. Equilibrium constants, solubility data, and reaction sets were defined to simulate impurity removal, particularly magnesium, and calcium salts. Laboratory-scale data were used to validate feed composition and preliminary operating conditions. Process performance was evaluated through mass and energy balances, product composition analysis and sensitivity studies on key operating variables such as reagent dosage, water addition, vapor flow rates and drying conditions. The simulation results indicate that the process achieves a final sodium chloride purity of approximately 98.3% by mass, suitable for industrial textile use, with an overall process yield of 93.3%. Sensitivity analysis identified optimal operating regions that maximize purity while minimizing reagent and energy consumption.*

**Keywords**— *Salt purification, textile industry, Aspen Plus, electrolyte simulation, sensitivity analysis.*

## INTRODUCTION

Sodium chloride (NaCl) is a fundamental raw material in numerous industrial processes, particularly in the textile industry, where it is extensively used in dyeing operations, reactive dye fixation, and chemical fiber treatments [1]. In the reactive dyeing of cellulosic fibers, NaCl acts as an electrolyte that neutralizes the negative zeta potential of the fiber, facilitating the adsorption of anionic dyes through electrostatic screening and thereby enhancing dye uptake efficiency [2].

However, insufficiently purified NaCl may contain significant amounts of divalent cations, mainly calcium and magnesium, which increase the hardness of the aqueous medium during dyeing. Experimental studies have shown that elevated water hardness negatively affects dyeing performance on cellulosic substrates, resulting in reduced dye uptake. This relationship is non-linear, reflecting the complex interference

of  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  ions with the dyeing process [3]. Consequently, these ions reduce color uniformity and overall process efficiency, increasing the need for chemical adjustments and operational costs.

On the other hand, when high-purity NaCl is used, dye exhaustion rates can increase to approximately 65–70%; however, it requires high salt dosages, typically ranging from 15 to 60 g/L in the dye bath and representing up to 100% of the fabric weight processed [2], [4]. As a result, reactive dyeing operations consume hundreds of thousands of tons of NaCl annually worldwide, significantly contributing to the saline load of textile effluents [4], [5].

The management of these salt-rich effluents constitutes one of the main environmental challenges faced by the textile sector, particularly in developing countries where technological and regulatory limitations hinder adequate wastewater treatment [5]. Despite these environmental challenges, the textile industry remains a key driver of industrial and economic growth, with a global market value exceeding USD 2 trillion and a strong dependence on chemical inputs such as NaCl [6], [7].

In Honduras, the textile industry accounts for approximately 4% of the national Gross Domestic Product, generates more than 139,000 direct jobs, and contributes exports exceeding USD 5.3 billion, consolidating its position as one of the country's most significant industrial sectors [8]. Within the manufacturing subsector, textile production represents over 95% of the economic activities associated with garment manufacturing, further reinforcing its strategic role in the national economy [8].

In parallel, artisanal saltworks in southern Honduras constitute an important source of local employment; however, limited infrastructure and low technological development constrain production capacity and hinder compliance with the purity standards required by the chemical and textile industries [9]. This situation presents an opportunity for the development of industrial processes aimed at marine salt purification to produce high-purity NaCl with added value, thereby strengthening the national value chain [9].

Process simulation using platforms such as Aspen Plus provides a robust framework for evaluating salt purification system design by integrating mass and energy balances,

thermodynamic modeling, and unit operation analysis. These tools enable systematic assessment of process performance under varying operating conditions, support early-stage design decisions, and reduce uncertainty in scale-up. Additionally, cost estimation and sensitivity analysis of key operating variables enable a comprehensive evaluation of both technical performance and preliminary economic feasibility.

Evaporation–crystallization processes for saline streams have been extensively modeled in Aspen Plus for salt recovery and purification applications. However, most reported studies focus on synthetic or industrial brines, with limited consideration of feedstocks exhibiting region-specific impurity characteristics and process variability.

The present work addresses this gap by integrating experimental data from artisanal marine salt production in Honduras with high-fidelity electrolyte simulation. Unlike conventional approaches, the proposed framework accounts for feedstock with unique impurity profiles (high  $Mg^{2+}/Ca^{2+}$  ratios) and variability typical of the region through electrolyte thermodynamic modeling (ELECNRTL). Coupled with sensitivity-driven analysis, the model identifies feasible operating windows for industrial-scale implementation.

## II. METHODOLOGY

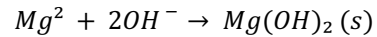
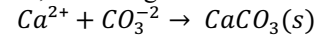
### A. Laboratory Work

The laboratory work aimed to obtain data from Honduran sea salt and to define the operating ranges of the main process variables, ensuring that the Aspen Plus simulation was developed on an experimental basis. Characterization tests were conducted on sea salt samples collected from artisanal saltworks in Honduras. Their physical and chemical properties were measured, including moisture content, saturated solution density, total hardness, particle size distribution, chemical composition, and mass flow rates. The experimental results were used as input parameters to define and adjust the salt feed stream (SAL-1-1) in the Aspen Plus model, as summarized in Table I.

TABLE I  
Physicochemical Characterization of Salt from Honduran Artisanal Saltworks

| Property                   | Experimental Value                                                                                          |
|----------------------------|-------------------------------------------------------------------------------------------------------------|
| Moisture                   | 2-2.09%                                                                                                     |
| Density                    | 1.026–1.027 g/mL.                                                                                           |
| Hardness                   | 1116.96 ppm expressed as $CaCO_3$                                                                           |
| Particle size distribution | Reduction of the fraction >10 mm from 44.9% to 18.0% after milling; 78.7% of the salt in the 10–18 mm range |
| Mass flow rate             | 5775 kg/h.                                                                                                  |
| Composition                | H <sub>2</sub> O 0.04<br>NaCl 0.8844<br>KCl 0.0275<br>MgCl <sub>2</sub> 0.0321<br>CaCl <sub>2</sub> 0.016   |

The dissolution time and the effect of particle size were evaluated. Laboratory milling achieved a representative dissolution time ( $\approx 59$  s at 100 rpm) and a sieving profile that was scaled to the proposed centrifugal mill. Chemical precipitation tests were conducted to remove the main impurities ( $Ca^{2+}$  and  $Mg^{2+}$ ) through the controlled addition of NaOH and  $Na_2CO_3$ , according to the reactions:



At a laboratory scale of 1 L, reagents were added and the precipitation of  $Mg(OH)_2$  and  $CaCO_3$  was observed. The experimentally determined amount to be added were approximately 5 mL of NaOH per 100 mL of brine and 2.5 mL of  $Na_2CO_3$  per 100 mL of brine. When scaled up, these values corresponded to estimated industrial consumptions of 432.6 L/h of 50% NaOH and 437.2 kg/h of  $Na_2CO_3$ . Finally, the settling velocity ( $\approx 2.5 \times 10^{-5}$  m/s) and cake characteristics were measured.

### B. Setting Properties on Aspen Plus

Since the studied system involves concentrated aqueous solutions of sodium chloride and the presence of ionic species responsible for hardness ( $Ca^{2+}$  and  $Mg^{2+}$ ), a thermodynamic model capable of accurately describing ion/ion and ion/solvent interactions. For this purpose, the ELECNRTL (Electrolyte Non-Random Two-Liquid) model was selected, which is widely used in the simulation of aqueous electrolyte solutions. This model combines the NRTL theory for molecular interactions with specific formulations for ionic species, allowing for a rigorous representation of phase equilibria, activity coefficients, and dissociation and precipitation phenomena in saline systems [10].

The selection of the ELECNRTL model is supported by its extensive development and validation for highly non-ideal aqueous electrolyte systems reported in the literature. The generalized formulation proposed by Chen and Song [11] enables rigorous prediction of activity coefficients over the entire concentration range, from dilute solutions to saturation conditions. The model has been independently validated using experimental mean ionic activity coefficient data for binary salt–water systems, including NaCl, KCl,  $MgCl_2$ , and  $CaCl_2$  [12], and has also been successfully implemented in Aspen Plus simulations of evaporative crystallization processes involving comparable saline streams [13]. In this study, the predicted solubilities of NaCl and KCl were additionally compared with the experimental solubility data reported in Perry's Chemical Engineers' Handbook [14], showing deviations consistent with those previously reported for ELECNRTL in multicomponent salt–water systems [12]. These results confirm the suitability of the model for representing the NaCl–KCl– $CaCl_2$ – $MgCl_2$ –H<sub>2</sub>O system evaluated in this work.

The solid and ionic components were defined, along with the dissociation and precipitation reactions, which were

classified as dissociation and salt reactions. The hardness removal reactions considered in this study were modeled under the assumption of chemical equilibrium, since the precipitation reactions of calcium and magnesium carbonates and hydroxides occur rapidly in aqueous systems and are primarily governed by thermodynamics constraints. In Aspen Plus, these reactions were solved using temperature-dependent equilibrium constants. A polynomial model for the equilibrium constant already existed (1), and the coefficients (A, B, C, D) were obtained by fitting solubility data from the Perry's Chemical Engineers' Handbook in Excel (Table II). These fitted coefficients were then used in Aspen Plus to calculate the temperature-dependent equilibrium constants.

$$\ln(K_{ps}) = A + \frac{B}{C} + C * \ln(T) + D * T + E \frac{(P - P_{ref})}{P_{ref}} \quad (1)$$

TABLE II  
Linearized Regression Coefficients for the Ksp Determination

| Reagent             | A        | B         | C        | D       |
|---------------------|----------|-----------|----------|---------|
| NaCl                | 108.1499 | -2486.693 | -18.778  | 0.036   |
| MgCl <sub>2</sub>   | 326.687  | -7392.32  | -58.465  | 0.119   |
| KCl                 | 432.151  | -13730.57 | -72.831  | 0.10716 |
| Ca(OH) <sub>2</sub> | 779.195  | -24169.62 | -132.098 | 0.1490  |

Coefficients obtained from linear regression of solubility data reported in Perry's Chemical Engineers' Handbook.

### C. Process Description

The process was modeled sequentially including brine pretreatment through dilution and mixing (Fig. 1). The stream SAL-1-1, representing raw sea salt, is combined with stream H2O-1-2 in mixer MX1-1-1 to obtain a homogeneous sodium chloride solution. This stage allows control of the initial brine

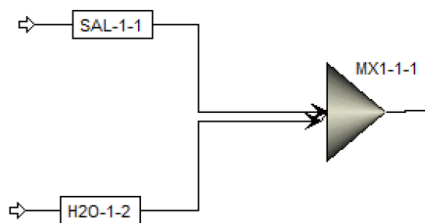


Fig. 1 Zone 1: Pretreatment

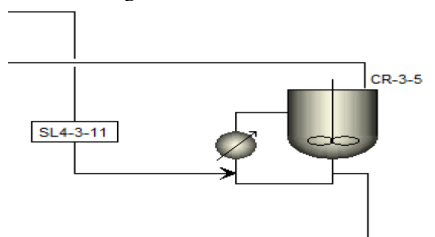


Fig. 3 Zone 3: Vacuum Crystallization

concentration and defines the ionic conditions entering the process, ensuring chemical stability in subsequent stages.

The process continues with chemical coagulation for impurity precipitation, followed by solid-liquid filtration and energy recovery via heat exchange (Fig. 2); Hardness removal is achieved through chemical precipitation. The brine from pretreatment is fed to mixer MX2-2-2, where streams NAOH-2-3 and NCO3-2-4, corresponding to sodium hydroxide and sodium carbonate, are added. These additions promote the precipitation of calcium and magnesium ions as CaCO<sub>3</sub>(s) and Mg(OH)<sub>2</sub>(s). The resulting stream SL2-2-6 is sent to filter FL1-2-3, where the precipitated solids are separated, producing DSOL-2-7 as a solid by-product. Subsequently, the liquid phase is thermally conditioned in heat exchanger INT-2-4, using steam streams CV-2-9 and VP2-2-10, to adjust the operating conditions prior to crystallization. Vacuum crystallization is then performed for the formation of solid NaCl occurs (Fig. 3). Stream SL4-3-11, originating from chemical coagulation stage feeds crystallizer CR-3-5, which operates under vacuum conditions. Pressure reduction promotes solvent evaporation and brine supersaturation, enabling controlled formation of NaCl crystals with lower dissolved impurities.

Finally, centrifugation is used for phase separation, followed by convective drying to obtain the final product (Fig. 4). The suspension from the crystallizer is fed to centrifuge CF-4-6, where wet salt (NWT-4-12) is separated from the residual liquid (LQF-4-13). The wet salt is transported via stream PRN-4-14 to dryer SC-4-7, where its moisture content is reduced using hot air (ARH-4-15) and cold air (ARC-4-16). The final stream SAL-4-17 represents the purified and dried salt, suitable for use in the textile industry. For each unit operation, the operating conditions, design parameters, and appropriate separation models were specified (Table III).

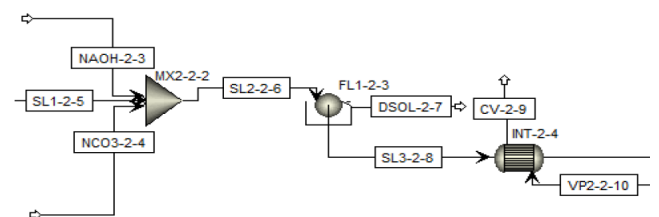


Fig. 2 Zone 2: Chemical Coagulation and Solid-Liquid Separation

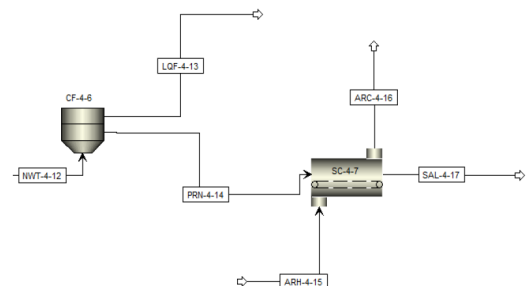


Fig. 4 Zone 4: Centrifugation and Convective Drying

TABLE III  
Unit Operation Parameters set On Aspen Plus

| Unit Operation | Description                                   | Temperature (°C) | Pressure (bar) | State        |
|----------------|-----------------------------------------------|------------------|----------------|--------------|
| MX1-1-1        | Mixer 1, Zone 1, Unit 1                       | 25               | 1              | Solid-Liquid |
| MX2-2-2        | Mixer 2, Zone 2, Unit 2                       | 25               | 1              | Solid-Liquid |
| FL1-2-3        | Filter, Zone 2, Unit 3                        | 25               | 1              | Solid-Liquid |
| INT-2-4        | Countercurrent Heat Exchanger, Zone 2, Unit 4 | 80               | 1              | Vapor-Liquid |
| CR-3-5         | Vacuum Crystallizer, Zone 3, Unit 5           | 25               | 0.5            | Vapor-Liquid |
| CF-4-6         | Centrifuge, Zone 4, Unit 6                    | 25               | 0.5            | Solid-Liquid |
| SC-4-7         | Convective Dryer, Zone 4, Unit 7              | 25               | 1              | Vapor-Liquid |

#### D. Setting Stream Parameters

Each stream in the sea salt purification process is characterized by its mass flow rate, composition, and physical state (Table IV). As illustrated in Fig. 5, the feed stream SAL-1-1 consists of a solid-liquid mixture of raw sea salt, while H2O-1-2 corresponds to liquid water used for dilution and brine homogenization. After chemical coagulation, stream SL2-2-6 represents a liquid brine depleted of divalent ions, whereas DSOL-2-7 is a solid by-product containing precipitated  $\text{CaCO}_3$  and  $\text{Mg(OH)}_2$ . The supersaturated brine SL4-3-11 enters the vacuum crystallizer, where the solid fraction forms NWT-4-12, a wet NaCl product with residual moisture, and LQF-4-13, the

remaining liquid containing non-crystallized salts and soluble impurities. The wet salt is transported via PRN-4-14 to the dryer, producing the final stream SAL-4-17, a dry and purified NaCl product. Key parameters for each stream include mass flow rate (kg/h), temperature, pressure, moisture content, and ionic composition, which were specified to ensure optimal separation efficiency, high NaCl recovery, and consistent product purity.

TABLE IV  
Stream Operation Parameters

| Stream                | State        | Temperature (°C) | Pressure (bar) | Mass Flow (kg/h) | Description                                           |
|-----------------------|--------------|------------------|----------------|------------------|-------------------------------------------------------|
| S. In SAL-1-1         | Solid-Liquid | 25               | 1              | 5775             | Raw sea salt, Zone 1, Stream 1                        |
| S. In H2O-1-2         | Liquid       | 25               | 1              | 14054            | Process water, Zone 1, Stream 2                       |
| S. In NaOH-2-3        | Solid-Liquid | 25               | 1              | 313              | Sodium hydroxide, Zone 2, Stream 3                    |
| S. In NCO3-2-4        | Solid        | 25               | 1              | 201              | Sodium carbonate, Zone 2, Stream 4                    |
| S. Pretreated SL1-2-5 | Solid-Liquid | 26.4             | 1              | 19829            | Solution 1, Zone 2, Stream 5                          |
| S. In SL2-2-6         | Solid-Liquid | 28.21            | 1              | 20343            | Solution 2, Zone 2, Stream 6                          |
| S. In DSOL2-7         | Solid-Liquid | 25               | 1              | 1244.47          | Precipitated solids, Zone 2, Stream 7                 |
| S. In SL3-2-8         | Solid-Liquid | 25               | 1              | 19098.5          | Solution 3, Zone 2, Stream 8                          |
| S. In VP2-2-10        | Vapor        | 100.122          | 0.5            | 13510            | Steam 1, Zone 2, Stream 9                             |
| S. Out CV2-9          | Vapor-Liquid | 81.31            | 0.5            | 13510            | Steam 2, Zone 2, Stream 10                            |
| S. In SL4-3-11        | Liquid       | 80               | 1              | 19098.5          | Solution 4, Zone 3, Stream 11                         |
| S. In NWT4-12         | Solid-Liquid | 100.122          | 0.5            | 5588.58          | Wet salt (NaCl brine), Zone 4, Stream 12              |
| S. In LQF4-13         | Liquid       | 100.122          | 1.013          | 285.077          | Final liquid (Mother liquor), Zone 4, Stream 13       |
| S. In PRN-4-14        | Solid        | 100.669          | 1.013          | 5303.5           | Purified salt (Concentrated brine), Zone 4, Stream 14 |
| S. In ARH-4-15        | Gas          | 150              | 1.013          | 110              | Hot air, Zone 4, Stream 15                            |
| S. Out ARC-4-16       | Gas          | 116.792          | 1.013          | 131.39           | Cold air, Zone 4, Stream 16                           |
| S. Out SAL-4-17       | Solid        | 91.0754          | 1.013          | 5282.11          | Final purified salt (NaCl product), Zone 4, Stream 17 |

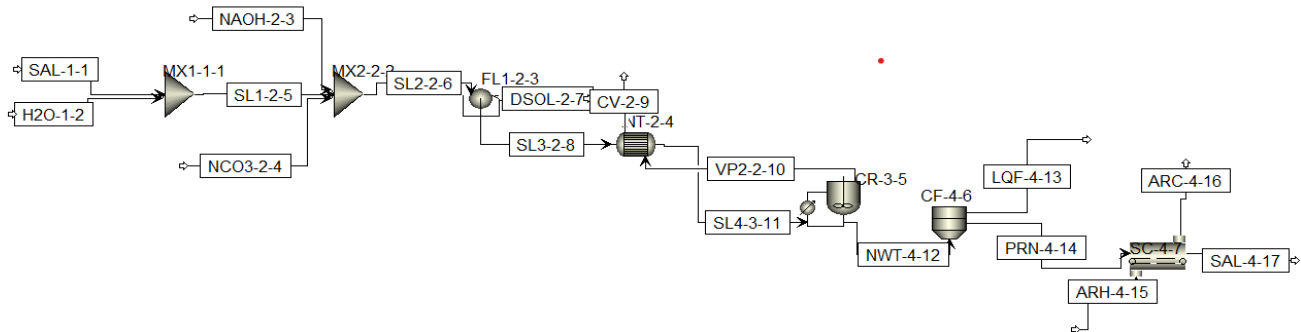


Fig. 5. Production of 98% Pure NaCl Process Flow Diagram Modeled in Aspen Plus.

#### E. Sensitivity Analysis in Aspen Plus

Four sensitivity analyses were performed within the simulation framework to determine the optimal operating conditions of key process stages. These analyses are described as follows:

**S1: Sensitivity analysis on MX1-1-1 (Fig. 6).** In this analysis, the mass flow rate of water added to mixer MX1-1-1 was varied to ensure complete dissolution of NaCl in the outlet brine. As shown in Fig. 6, the undissolved NaCl decreases sharply with increasing water flow rate, reaching zero at approximately 14,040 kg/h. Beyond this point, additional water does not improve dissolution, indicating that complete solubilization has already been achieved. Therefore, this value represents the minimum dilution requirement, and further water addition would only increase process volume and energy demand without improving performance

**S2: Sensitivity analysis on CR-3-5 (Fig. 7).** In this analysis, the mass flow rate of vapor leaving the crystallizer was varied to evaluate its effect on NaCl precipitation and impurity incorporation. As illustrated in Fig. 7, increasing vapor flow enhances NaCl crystallization due to higher supersaturation, resulting in increased NaCl mass fraction in the solid phase. However, excessive vapor removal may also influence the distribution of impurities such as KCl. This behavior highlights the existence of an optimal operating range, where NaCl recovery is maximized while minimizing impurity incorporation and avoiding unnecessary energy consumption.

**S3: Sensitivity analysis on MX2-2-2 (Fig. 8)** In this case, the mass flow rate of NaOH added to mixer MX2-2-2 was varied to assess its effect on magnesium removal. As shown in Fig. 8, the mass fraction of dissolved  $Mg^{2+}$  decreases rapidly

with increasing NaOH dosage, approaching negligible values at relatively low flow rates. Beyond this point, further NaOH addition does not significantly improve magnesium removal, indicating that the precipitation of  $Mg(OH)_2$  is effectively complete. Therefore, an optimal NaOH dosage can be defined to minimize reagent consumption while achieving efficient impurity removal.

**S4: Sensitivity analysis on MX2-2-2 (Fig. 9)** Similarly, the mass flow rate of  $Na_2CO_3$  was varied to evaluate its effect on calcium removal through  $CaCO_3$  precipitation. As shown in Fig. 9, increasing  $Na_2CO_3$  dosage reduces the mass fraction of dissolved  $Ca^{2+}$ ; however, the rate of reduction decreases progressively, indicating diminishing returns at higher dosages. This trend suggests that calcium removal follows an asymptotic behavior, and excessive reagent addition leads to marginal improvements while increasing operational costs. Consequently, an optimal dosage must balance removal efficiency and economic performance.

The selection of these analyses was aimed at identifying optimal operating conditions that balance NaCl purity with energy and reagent consumption. Variables such as product purity, specific steam consumption (kg steam/kg salt produced), and chemical reagent dosage were evaluated simultaneously. The results indicate that while increased steam flow enhances NaCl purity through improved crystallization, it also significantly increases energy demand. Similarly, higher reagent dosages improve impurity removal but exhibit diminishing returns, leading to higher operating costs. These findings highlight the importance of defining optimal operating windows rather than maximizing individual variables.

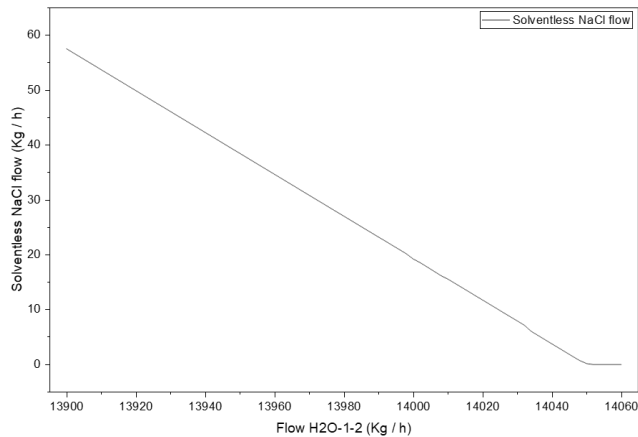


Fig. 6 Effect of dilution water flow rate on NaCl dissolution at the outlet of mixer MX1-1-1.

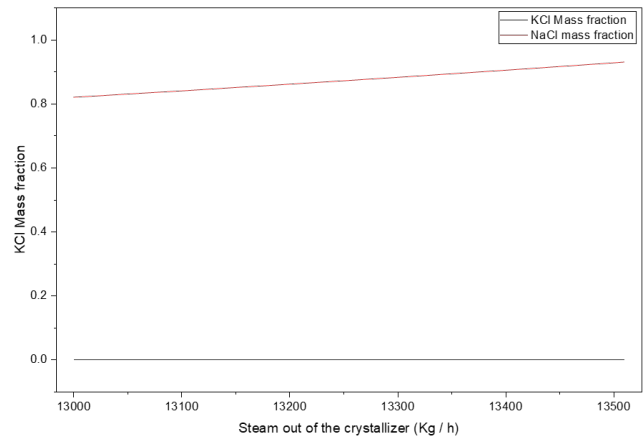


Fig. 7 Effect of vapor flow rate on NaCl precipitation and impurity formation in the vacuum crystallizer.

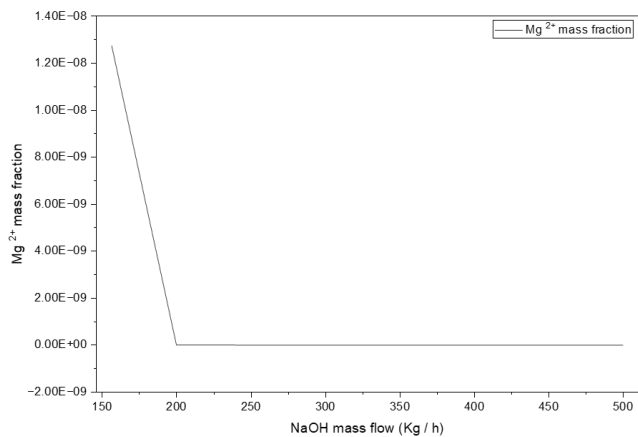


Fig. 8 Influence of NaOH flow rate on dissolved magnesium concentration at the outlet of mixer MX2-2-2.

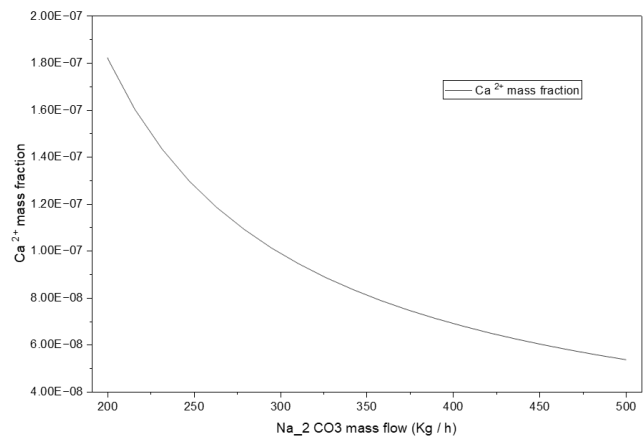


Fig. 9. Effect of  $\text{Na}_2\text{CO}_3$  flow rate on dissolved calcium concentration at the outlet of mixer MX2-2-2.

### III. RESULTS AND EFFICIENCY

The simulation of the integrated sea salt purification process in Aspen Plus (Fig. 5) enabled a detailed assessment of production performance, product quality, and overall process efficiency. Under the optimal operating conditions identified through sensitivity analysis, the process achieved a total annual solid production of 50,978.7 t/year, of which 50,113.6 t/year corresponds to sodium chloride (NaCl). This corresponds to an overall NaCl mass purity of 98.30 wt.% in the final product stream (SAL-4-17), indicating that the proposed process configuration can produce high-quality industrial salt suitable for textile applications.

Analysis of the product composition shows that NaCl is the dominant component of the solid phase, while impurities are present at relatively low levels. The primary impurity identified is potassium chloride (KCl), with an annual production of 293.687 t/year, representing approximately 0.58 wt.% of the total solids. Other species are present only in trace amounts: calcium chloride ( $\text{CaCl}_2$ ) appears at 0.00565 t/year, while magnesium hydroxide  $[\text{Mg}(\text{OH})_2]$  is absent from the final solid product, confirming the effectiveness of the chemical coagulation stage for magnesium removal. Minor quantities of  $\text{CaCO}_3$ , residual ions ( $\text{Cl}^-$ ,  $\text{Na}^+$ ), and carbonate species were detected at levels below 0.0005 wt.%, which are negligible from an industrial perspective and do not compromise product quality.

Further improvements in product purity could be achieved by incorporating a crystal washing stage using saturated NaCl solution (brine). This operation should be implemented after crystallization and before drying, with the objective of removing the mother liquor adhering to the crystal surface, which contains soluble impurities such as KCl.

NaCl crystals exit the crystallizer covered by a thin film of solution which, although in equilibrium with the solid phase, has a different composition enriched in impurities. To remove this film without significant product loss, washing with NaCl-saturated brine is employed. This solution is in equilibrium with solid NaCl, minimizing its dissolution while facilitating the removal of KCl and other more soluble salts present on the crystal surface. This washing step can be effectively implemented in a centrifuge by controlling the

flow rate of the wash brine, thereby enhancing final product purity, and reducing impurity content.

Global performance indicators further confirm the effectiveness of the process. Although the final NaCl purity does not exceed 99 wt.%, the achieved value of 98.3 wt.% represents high-grade industrial salt. The residual impurity content is primarily associated with KCl, which remains in solution due to its higher solubility and tendency to co-crystallize with NaCl. These results highlight a clear opportunity for future optimization focused on selective KCl removal without significantly affecting NaCl recovery. A detailed summary of the simulation results obtained from Aspen Plus is presented in Table V.

TABLE V  
Summary Table

| Parameter / Stream            | SAL-1-1  | H2O-1-2  | NaOH-2-3 | NCO3-2-4  | SL1-2-5   | SL2-2-6   | DSOL2-7    | SL3-2-8        | VP2-2-10 |
|-------------------------------|----------|----------|----------|-----------|-----------|-----------|------------|----------------|----------|
| Enthalpy Flow (Gcal/hr)       | -10.1547 | -53.2907 | -1.09    | -0.511466 | -63.4452  | -64.9766  | -4.01641   | -61.0075       | -42.8994 |
| Average MW                    | 53.6212  | 18.0153  | 18.9552  | 105.99    | 20.2270   | 20.3879   | 22.826     | 20.2473        | 18.0153  |
| Mole Flow (kmol/hr)           | 107.6990 | 780.116  | 16.5126  | 1.89643   | 980.321   | 997.797   | 54.5197    | 943.265        | 749.917  |
| Mass Flow (kg/hr)             | 5775     | 14054    | 313      | 201       | 19829     | 20343     | 1244.47    | 19098.5        | 131510   |
| H2O (mass frac)               | 0.0400   | 1        | 0.5      | 0         | 0.7204    | 0.7099    | 0.603437   | 0.7168         | 1        |
| NaCl (mass frac)              | 0.8844   | 0        | 0        | 0         | 0         | 0         | 3.0412E-05 | 3.62E-05       | 0        |
| KCl (mass frac)               | 0.0275   | 0        | 0        | 0         | 0         | 0         | 0          | 0              | 0        |
| NaOH (mass frac)              | 0        | 0        | 0.5      | 0         | 0         | 0         | 0          | 0              | 0        |
| Na2CO3 (mass frac)            | 0        | 0        | 0        | 1         | 0         | 0         | 0          | 0              | 0        |
| MgCl2 (mass frac)             | 0.0321   | 0        | 0        | 0         | 0         | 0         | 0          | 0              | 0        |
| CaCl2 (mass frac)             | 0.0160   | 0        | 0        | 0         | 0         | 0         | 0          | 0              | 0        |
| Mg(OH)2 (mass frac)           | 0        | 0        | 0        | 0         | 0         | 0         | 0.0912435  | 7.94E-10       | 0        |
| Cl <sup>-</sup> (mass frac)   | 0        | 0        | 0        | 0         | 0.1700    | 0.1957    | 0.140836   | 0.1673         | 0        |
| Na <sup>+</sup> (mass frac)   | 0        | 0        | 0        | 0         | 0.1013    | 0.1075    | 0.0913     | 0.1085         | 0        |
| OH <sup>-</sup> (mass frac)   | 0        | 0        | 0        | 0         | 0         | 1.57E-05  | 1.33E-05   | 1.58E-05       | 0        |
| Co3 <sup>2+</sup> (mass frac) | 0        | 0        | 0        | 0         | 0         | 0.0031    | 0.0027     | 0.0032         | 0        |
| CaCo3 (mass frac)             | 0        | 0        | 0        | 0         | 0         | 0         | 0.0670     | 0              | 0        |
| K <sup>+</sup> (mass frac)    | 0        | 0        | 0        | 0         | 0.0042    | 0.0041    | 0.0035     | 0.0041         | 0        |
| Mg2 <sup>+</sup> (mass frac)  | 0        | 0        | 0        | 0         | 0.0024    | 1.27E-08  | 1.05E-08   | 1.25E-08       | 0        |
| Ca2 <sup>+</sup> (mass frac)  | 0        | 0        | 0        | 0         | 0.0017    | 1.81E-07  | 1.57E-07   | 1.82E-07       | 0        |
| Air (mass frac)               | 0        | 0        | 0        | 0         | 0         | 0         | 0          | 0              | 0        |
|                               | CV2-9    | SL4-3-11 | NWT4-125 | LQF4-13   | PRN-4-14  | ARC-4-16  | ARH-4-15   | SAL-4-17       | -        |
| Enthalpy Flow (Gcal/hr)       | -43.6588 | -60.2431 | -9.7165  | -0.774004 | -8.94195  | -0.108625 | -0.0193677 | -8.85515       | -        |
| Average MW                    | 18.0153  | 20.2047  | 53.5163  | 25.243    | 56.8824   | 25.8394   | 28.0981    | 57.7357        | -        |
| Mole Flow (kmol/hr)           | 749.917  | 943.276  | 104.4280 | 11.2933   | 93.2363   | 6.87959   | 5.33844    | 91.3773        | -        |
| Mass Flow (kg/hr)             | 13510    | 19098.5  | 5588.58  | 285.077   | 5303.5    | 177.764   | 150        | 5275.73        | -        |
| H2O (mass frac)               | 1        | 0.7168   | 0.0323   | 0.46168   | 0.0092336 | 0.198376  | 0.05       | 0.0040197<br>1 | -        |
| NaCl (mass frac)              | 0        | 0        | 0.9300   | 0         | 0.97909   | 0         | 0          | 0.983031       | -        |

|                                             |   |          |          |          |            |        |      |             |   |
|---------------------------------------------|---|----------|----------|----------|------------|--------|------|-------------|---|
| KCl (mass frac)                             | 0 | 0        | 0        | 0        | 0.0009978  | 0      | 0    | 0.00576098  | - |
| NaOH (mass frac)                            | 0 | 0        | 0        | 0        | 0          | 0      | 0    | 0           | - |
| Na <sub>2</sub> CO <sub>3</sub> (mass frac) | 0 | 0        | 0        | 0        | 0          | 0      | 0    | 0           | - |
| MgCl <sub>2</sub> (mass frac)               | 0 | 0        | 0        | 0        | 0          | 0      | 0    | 0           | - |
| CaCl <sub>2</sub> (mass frac)               | 0 | 0        | 0        | 0        | 0          | 0      | 0    | 0           | - |
| Mg(OH) <sub>2</sub> (mass frac)             | 0 | 9.98E-10 | 1.05E-05 | 0        | 1.1113E-07 | 0      | 0    | 1.11714E-07 | - |
| Cl <sup>-</sup> (mass frac)                 | 0 | 0.1673   | 0.0076   | 0.109226 | 0.00286653 | 0      | 0    | 0.000745225 | - |
| Na <sup>+</sup> (mass frac)                 | 0 | 0.1085   | 0.0050   | 0.0717   | 0.0029     | 0      | 0    | 0.0023      | - |
| OH <sup>-</sup> (mass frac)                 | 0 | 1.58E-05 | 5.40E-05 | 0.0008   | 0.0022     | 0      | 0    | 1.55E-05    | - |
| Co <sub>3</sub> <sup>^2</sup> (mass frac)   | 0 | 0.0032   | 0.0108   | 0.1547   | 1.54E-05   | 0      | 0    | 0.0031      | - |
| CaCo <sub>3</sub> (mass frac)               | 0 | 1.60E-07 | 1.56E-06 | 0        | 1.64E-06   | 0      | 0    | 1.65E-06    | - |
| K <sup>+</sup> (mass frac)                  | 0 | 0.0041   | 0.0141   | 0.2019   | 0.0035     | 0      | 0    | 0.0010      | - |
| Mg <sub>2</sub> <sup>+</sup> (mass frac)    | 0 | 1.24E-08 | 8.24E-13 | 1.18E-11 | 1.28E-13   | 0      | 0    | 4.28E-14    | - |
| Ca <sub>2</sub> <sup>+</sup> (mass frac)    | 0 | 1.18E-07 | 2.17E-11 | 3.10E-10 | 9.80E-12   | 0      | 0    | 1.26E-11    | - |
| Air (mass frac)                             | 0 | 0        | 0        | 0        | 0          | 0.8016 | 0.95 | 0           | - |

The overall efficiency of the process was evaluated based on the conversion of chloride ions (Cl<sup>-</sup>), considered the limiting species, into solid NaCl. From the feed stream SL1-2-5, a chloride flow of 95.0815 kmol/h enters the system. In the final product stream SAL-4-17, the NaCl production corresponds to 88.7404 kmol/h, resulting in an overall process efficiency of 93.33% (2). This high conversion indicates that most of the available chloride is effectively recovered as solid NaCl, with limited losses to liquid waste streams.

$$\%E = \frac{88.7404}{95.0815} * 100\% = 93.33\% \quad (2)$$

#### IV. DISCUSSION

The behavior observed in the simulated process can be explained by the physicochemical characteristics of multicomponent saline systems and the selected separation mechanisms. Chemical coagulation using NaOH and Na<sub>2</sub>CO<sub>3</sub> effectively targets divalent ions by converting calcium and magnesium into insoluble species, thereby reducing solution hardness, and stabilizing the ionic environment prior to crystallization [14]. This pretreatment step is critical, as the presence of Ca<sup>2+</sup> and Mg<sup>2+</sup> is known to interfere with crystal growth, promote scaling, and deteriorate product quality in industrial salt production. Their effective removal confirms the suitability of precipitation-based softening for saline purification processes.

In contrast, potassium remains largely unaffected by coagulation due to its high solubility and chemical similarity to sodium. The persistence of KCl is therefore governed by thermodynamic limitations rather than process inefficiencies. Under the operating conditions evaluated, the activity coefficients and solubility behavior of KCl closely resemble those of NaCl, resulting in partial co-crystallization [15]. This phenomenon is typical in saline crystallization systems and

highlights an inherent limitation of single-stage crystallization when treating potassium-containing brines. Consequently, further reduction of potassium content would require separation strategies based on differential solubility, such as fractional crystallization or controlled washing, rather than chemical treatment [16]. This behavior is consistent with multicomponent saline systems, where process selectivity is governed by differences in solubility and crystallization kinetics [17].

Vacuum crystallization was shown to be a decisive unit operation in defining product quality, as reduced pressure allows crystallization at lower temperatures, limiting thermal degradation and enabling finer control of supersaturation. Operating near the metastable zone boundary favors NaCl crystal growth while constraining impurity incorporation, demonstrating the importance of thermodynamic control in salt purification processes [18]. The sensitivity of product quality to vapor flow reinforces the need for precise energy and phase equilibrium management in industrial crystallizers.

It should also be noted that the precipitation and crystallization stages in this study were modeled under thermodynamic equilibrium assumptions, which are commonly applied to rapid precipitation reactions such as the formation of CaCO<sub>3</sub> and Mg(OH)<sub>2</sub> [19], [20]. However, crystallization processes are governed not only by thermodynamic driving forces but also by kinetic mechanisms, including nucleation and crystal growth, both of which are strongly influenced by supersaturation levels and system hydrodynamics [21], [22]. Recent atomistic studies have demonstrated that NaCl crystallization can transition from a one-step to a two-step nucleation mechanism upon crossing the spinodal limit [22], while confinement effects and local kinetic conditions may promote the formation of transient amorphous intermediates [21]. At the industrial

scale, evaporative crystallization of NaCl has been experimentally observed to nucleate at lower supersaturation levels in larger vessels compared to microscale systems [23]. Similarly,  $\text{Mg}(\text{OH})_2$  precipitation from real sea bittern has shown significantly different nucleation and growth coefficients than those obtained from synthetic solutions [20]. In addition, foreign ions such as  $\text{K}^+$  and  $\text{Na}^+$ , which are present in the studied brine, can alter the crystallization pathway and kinetics of  $\text{CaCO}_3$  formation [24]. These kinetic effects may influence crystal size distribution, impurity incorporation, and overall separation efficiency, particularly during scale-up from laboratory to industrial operation. Therefore, the equilibrium framework adopted in this work provides a robust upper-bound approximation of separation performance, whereas a fully predictive industrial model would require coupling population balance equations with kinetic rate expressions [19], [20].

The resulting configuration led to a total capital expenditure (CAPEX) of approximately 7.13 million USD for the proposed system, as estimated through a preliminary economic assessment using Aspen Process Economic Analyzer (APEA). This CAPEX reflects the full integration of the unit operations defined in the Aspen Plus model, including mixing, chemical precipitation, solid-liquid separation, vacuum crystallization, centrifugation, and drying stages.

The estimated total operating expenditure (OPEX) is approximately 7.19 million USD per year, as obtained from the simulation-based economic analysis. This value is primarily driven by raw material consumption, particularly the marine salt feed (5775 kg/h), as well as the use of chemical reagents such as sodium hydroxide (313 kg/h) and sodium carbonate (201 kg/h) required for hardness removal.

Additional contributions to operating costs arise from utility demands, including water usage (14,054 kg/h) and energy consumption associated with thermal operations. Energy consumption in the process is primarily concentrated in the vacuum crystallization stage. Aspen Plus results indicate that the crystallizer operates at 0.5 bar and 100.12 °C, with a calculated heater duty of 7.63 Gcal/h and a vapor generation rate of 13,510 kg/h, confirming that this unit represents the dominant thermal load due to its evaporation-driven mechanism for supersaturation generation.

In contrast, the convective drying stage functions mainly as a final moisture-reduction step rather than a major evaporation unit. In this case, thermal energy is supplied through the hot air stream rather than as an explicit external heat duty. The energy required for moisture removal is therefore embedded in the enthalpy of the inlet air stream and transferred to the solids during drying. This behavior is supported by the enthalpy values reported in Table V, where

the inlet air stream (ARH-4-15) and outlet air stream (ARC-4-16) show a change in enthalpy flow from  $-0.0194$  to  $-0.1086$  Gcal/h, respectively. The decrease in air temperature from the inlet to the exhaust stream, together with the increase in moisture content, confirms that effective heat and mass transfer are taking place within the unit.

From an industrial perspective, these results indicate that the overall thermal feasibility of the process is governed mainly by the crystallization stage, while the drying step contributes a comparatively lower energy demand under the modeled conditions. This is consistent with industrial crystallization systems, where evaporation and supersaturation control represent the primary energy requirements of the process [25]. Additionally, the process incorporates internal heat recovery by reusing the vapor generated in the crystallizer (CR-3-5) as the heating medium in the upstream heat exchanger (INT-2-4), improving overall thermal efficiency.

## V. CONCLUSIONS

The integrated simulation of the sea salt purification process using Aspen Plus confirms the technical feasibility of producing high-quality industrial sodium chloride through a combination of pretreatment, chemical coagulation, vacuum crystallization, centrifugation, and drying. The proposed configuration achieves an effective balance between impurity removal, product recovery, and operational simplicity, supporting its potential for large-scale implementation.

Chemical coagulation proved to be a critical step for hardness removal, stabilizing brine composition and enabling efficient downstream crystallization. The effective precipitation of  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  minimized their interference with crystal growth, while vacuum crystallization provided the thermodynamic conditions required to promote NaCl formation with limited impurity incorporation. The integration of solid-liquid separation and controlled drying ensured a consistent final product with low residual moisture, reinforcing the robustness of the overall process design.

The process achieved a NaCl purity of approximately 98.3 wt.% and an overall recovery of 93.3%, confirming its suitability for industrial textile applications, where consistent composition and low hardness are essential. The remaining presence of potassium-based impurities is attributed to inherent thermodynamic limitations of multicomponent saline systems, particularly the similarity in solubility behavior between NaCl and KCl, rather than to process inefficiencies.

From a preliminary economic perspective, the estimated capital investment of approximately 7.13 million USD reflects the integration of the main unit operations required

for industrial implementation. Operating costs are primarily driven by raw material consumption and thermal energy demand, particularly in the vacuum crystallization stage, which represents the dominant energy load of the process. While these estimates provide a useful indication of economic feasibility, they remain subject to the assumptions inherent to the simulation model and should be further refined through detailed design and experimental validation.

Overall, the results highlight the importance of defining optimal operating conditions that balance product purity, energy consumption, and reagent usage, rather than maximizing individual variables. This approach enables a more efficient and scalable process design for industrial salt purification.

Future work should focus on process intensification strategies, including selective potassium removal through washing or fractional crystallization, as well as optimization of energy integration in crystallization and drying stages. In addition, further studies should incorporate kinetic considerations of precipitation and crystallization processes, including nucleation and crystal growth rates, to complement the equilibrium-based approach used in this work. This would enable a more accurate representation of scaling behavior and facilitate the transition from laboratory-scale assumptions to industrial implementation.

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