



COMPOSITION-PROPERTY RELATIONSHIPS IN HIGH-SALINITY ARTIFICIAL SEAWATER: STATISTICAL ANALYSIS OF PH, CONDUCTIVITY, OSMOLALITY AND ELEMENTAL COMPOSITION

Joseph P. De Vera

Biology & GP Teacher, Biology, Department of STEM, Nurafshon Presidential School, Uzbekistan, Email: josephdevera.dlabbc@gmail.com, ORCID ID: 0009-0007-7484-7422

Received:-23/06/2025, Revised:-02/08/2026, Accepted:-12/09/2026, Published:-25/09/2026

ABSTRACT

High-salinity artificial seawater provides a controlled medium for examining how increasing dissolved salt concentrations alter chemical composition and potentially influence physicochemical behaviour. This study characterized compositional changes across artificial seawater formulations spanning 36,032–80,000 ppm total dissolved solids (TDS). Ten chemical constituents were evaluated, including NaCl, MgCl₂, Na₂SO₄, CaCl₂, KCl, NaHCO₃, KBr, B(OH)₃, SrCl₂, and NaF. Data were processed in Python using descriptive statistics, percentage composition, concentration differences, fold changes, and linear trend analysis. NaCl was consistently the dominant constituent, accounting for approximately 68% of total composition, followed by MgCl₂ and Na₂SO₄. The five major salts collectively represented approximately 99% of the formulation. Major constituent concentrations increased approximately 2.22-fold between the lowest and highest TDS conditions, while their relative proportions remained largely stable. The findings demonstrate controlled proportional enrichment across the salinity gradient and provide a compositional foundation for future evaluation of pH, conductivity, and osmolality. Direct physicochemical measurements will be necessary to establish these composition-property relationships experimentally.

KEYWORDS: *Artificial seawater, High salinity, Ionic composition, Total dissolved solids, Composition–*

1. INTRODUCTION

The High salinity aqueous systems play an important role in the fields of desalination, marine engineering, as well as wastewater management and control experiments with seawater, where the physicochemical behaviour is significantly influenced by the dissolved ionic composition. The growing interest in concentrated saline streams and their management is driven by growing industrial water demand, and expansion of desalination. Wastewater with high sodium content is especially problematic as the high salt content can lead to reduced efficiency of existing treatment processes and the demand for salt-specific treatment technologies (Li et al., 2025). Desalination technologies are a growing and valuable way to secure freshwater supplies, but are also impacted by key technical, energetic and concentrated residual streams management challenges (Wang & Huo, 2022).

Brine from desalination is an example of high salinity water system as the chemical composition of it is different from the chemistry of the environment to which it is being added. Adequate management of discharge can prevent the impact of concentrated salts and related constituents on local marine chemistry when they are discharged (Omerspahic et al., 2022). The same challenges are faced in high salinity wastewaters with high ionic strength and various dissolved species, where treatment and resource recovery will be more complicated (Guo et al., 2023). As a result, biological methods have been studied along with the physicochemical methods such as removal of pollutants, remediation and applications in desalination using algae (Hasnain et al., 2025). The knowledge of the chemical behaviour of concentrated salt solutions is thus of importance not only in terms of engineered treatment systems but also for environmental protection.

Total salinity is not an adequate parameter for seawater chemistry. Many of its measurable properties are determined by the presence of major ions in solution such as sodium, chloride, magnesium, calcium, potassium and sulfate. Environmental hydrochemical studies reveal the need to consider individual ions in addition to common water quality parameters when looking at water quality (Dharmapriya et al., 2023). Ionic signatures are also effective for the detection of seawater intrusion in freshwater aquifers, which salinizes the groundwater, and consequently affects the quality of the water (Ligori et al., 2025). Hydrochemical assessment also relies on comprehensive assessment of the dissolved constituents and the physicochemical characteristics to identify differences between water sources and environmental conditions (Oguntade, 2023).

Artificial seawater provides a controlled matrix of constituents concentrations which can be varied systematically while other experimental conditions are held constant to investigate these relationships. This type of control is especially useful at high salinity, because of possible interactions between dissolved species that could cause behaviour outside of that predicted for dilute solutions. The concentration and the interaction between molecules or ions in an aqueous electrolyte solution have an impact on the properties of the solution, and highly concentrated solutions are of particular interest in studying the deviation from the simple assumption of ideal solution (Zavitsas, 2022). Controlled composition–property analysis can hence elucidate if there are linear or more complex changes in measurable physicochemical properties associated with increases in total dissolved solids.

Of these properties, pH, electrical conductivity and osmolality are complementary aspects of solution behaviour. Conductivity is a measure of the ability of the ions in solution to conduct an electric charge, and pH is a measure of the acid–base properties of the water. The parameter osmolality is useful for giving a measure of the number of osmotically active dissolved species. Osmotic concentration is a well-known concept in fluid chemistry and physiology, where the distribution of water is greatly influenced by the concentration and location of dissolved substances (Henderson et al.,

2021). Clinical studies also show that osmolality or osmolarity can be calculated using certain dissolved components, but for different solution compositions, the calculated value may deviate from the directly determined value (Berska et al., 2023). The osmolality is therefore considered to be a valuable measure of the solute concentration and hyperosmolar states (Büyükkaragöz & Bakkaloğlu, 2023; Najem et al., 2024). These latter studies refer to biological fluids and not to seawater, but do bear on the methods used for the interpretation of osmotic concentration.

Other than the use of seawater in water treatment, the chemical composition of seawater has also practical implications. Marine structures are permanently exposed to the marine environment in which the saline solutions, corrosion processes and fouling occur and interact over a long period of time. Hence, the knowledge of the seawater composition is important in the prediction of the behaviour of the material and maintenance of the marine infrastructure (Vedaprakash et al., 2022). All of these applications illustrate that saline solutions should be characterized not only by their total salt content, but by the interrelationships between the various constituents and resulting physico-chemical properties.

In spite of the many studies on desalination, saline wastewater, hydrochemistry and osmotic behaviour, rather limited work has been performed on the statistical characterization of composition-property relationships in an integrated fashion, for different controlled high-salinity artificial seawater formulations. There are many investigations that focus upon one of the following areas: overall salinity, selected ions, environmental water quality, or individual physicochemical properties. A systematic relationship between changes in composition of the artificial seawater and pH, conductivity, osmolality, elemental or ionic profile could give more information on the concentrated seawater systems. To this end the study had three objectives:

- To characterize compositional variation across high-salinity artificial seawater formulations.
- To examine relationships between salinity, major ionic constituents, and physicochemical properties.
- To statistically identify dominant composition–property patterns across increasing salinity levels.

2.MATERIALS AND METHODS

2.1Study Design and Dataset

A quantitative analytical design was applied for the characterization of compositional variation of high salinity artificial seawater. The formulations ranged from 36,032 ppm to 80,000 ppm TDS which gave a controlled salinity gradient. Ten predefined chemical constituents were utilized in each formulation and these were in g/L. Changes in constituent concentrations, relative composition and concentration scaling with increasing salinity were used in the analysis.

2.2Artificial Seawater Composition

The compositions were made with NaCl, MgCl₂, Na₂SO₄, CaCl₂, KCl, NaHCO₃, KBr, B(OH)₃, SrCl₂, and NaF. Concentrations were calculated with constituent mass and preparation volume, and normalized to g/L. NaCl was the major component followed by MgCl₂ and Na₂SO₄. Concentrations of the different constituents were changed while maintaining the relative proportions of the constituents throughout the salinity gradient, allowing direct evaluation of the compositional changes with concentration.

2.3 Data Preparation and Quality Assessment

The data were checked for completeness, consistency and units of measurement prior to analysis. Individual component concentrations were normalized to g/L, and classified by target TDS. Concentrations of chemicals were added together for each formulation to get the total concentration of chemicals. The percentages of each constituent to the total concentration were taken as the relative composition. The absolute and fold changes were determined from the lowest to the highest salinity.

2.4 Composition–Salinity Assessment

Major constituents were assessed over the entire range of TDS, with special focus on NaCl, MgCl₂, Na₂SO₄, CaCl₂ and KCl. The salinity increase in each formulation was compared with concentration profiles and relative contributions to determine if the salinity increase affected the proportions of the chemicals or resulted in proportional enrichment. Absolute differences in concentrations and fold changes were used to quantify changes in the range of 36,032 – 80,000 ppm.

2.5 Statistical Analysis

Data analysis was done using pandas, NumPy and Matplotlib in Python. Chemical constituents were calculated in terms of descriptive statistics, percentage composition, absolute changes and fold changes. Linear trend analysis was used to determine the association between target TDS and total concentration of constituents. Graphical representations of the concentration profiles and the relative compositional distributions were made to describe systematic changes along the salinity gradient.

3. RESULTS

3.1 Composition of High-Salinity Artificial Seawater

Artificial seawater is composed of 3.1% of the following ingredients. The salinity range for the artificial seawater formulations was wide, from 36032 to 80000 ppm of TDS. Ten chemical constituents were found in all formulations, NaCl being the predominant salt in all. Table 1 shows that NaCl increased from 24.540 g/L at 36,032 ppm to 54.481 g/L at 80,000 ppm. The next most common constituents were MgCl₂, and Na₂SO₄. As can be seen in figure 1, the concentrations of major salts increase systematically as the TDS goes up due to progressive enrichment of the formulation series.

Table 1. Major Chemical Composition of Selected Artificial Seawater Formulations

TDS (ppm)	NaCl (g/L)	MgCl ₂ (g/L)	Na ₂ SO ₄ (g/L)	CaCl ₂ (g/L)	KCl (g/L)
36,032	24.540	5.200	4.100	1.160	0.695
40,000	27.260	5.777	4.550	1.289	0.772
50,000	34.048	7.218	5.677	1.610	0.965
60,000	40.867	8.663	6.814	1.933	1.158
70,000	47.670	10.104	7.950	2.254	1.350
80,000	54.481	11.549	9.084	2.576	1.544

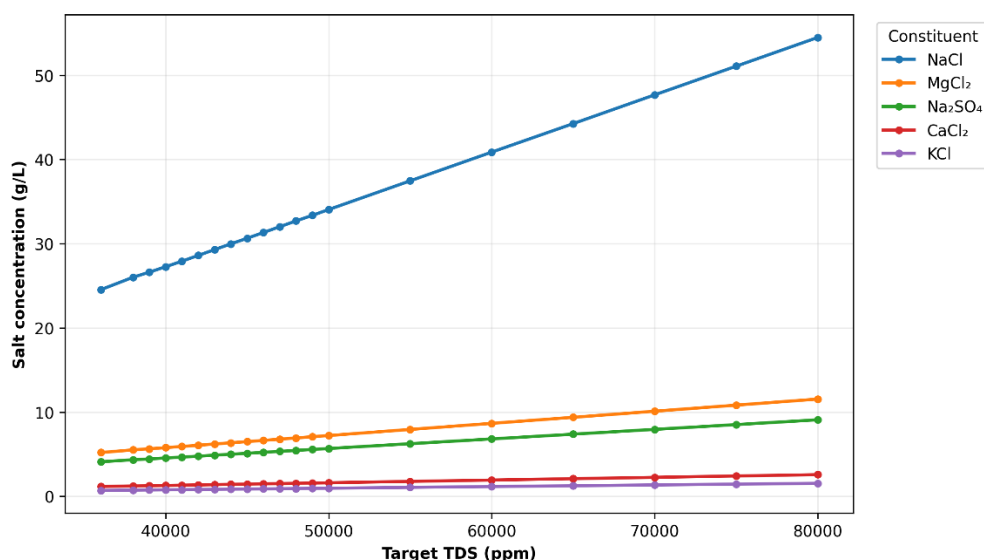


Figure 1. Variation in Major Salt Concentrations Across Artificial Seawater Salinity Levels

3.2 Relative Distribution of Chemical Constituents

Relative composition was very constant, even though there was a significant change in total salinity. Table 2 indicated that the concentration of NaCl was about 68.08% whereas MgCl_2 and Na_2SO_4 were 14.43% and 11.35% respectively. Smaller proportions of CaCl_2 and KCl were added. These 5 most important salts accounted for about 99% of the formulation. As seen in Fig. 2, at representative salinities the relative proportions of the constituents are preserved with NaCl dominating.

Table 2. Relative Contribution of Artificial Seawater Constituents

Constituent	Composition (%)	36,032 ppm (g/L)	80,000 ppm (g/L)
NaCl	68.08	24.540	54.481
MgCl_2	14.43	5.200	11.549
Na_2SO_4	11.35	4.100	9.084
CaCl_2	3.22	1.160	2.576
KCl	1.93	0.695	1.544
NaHCO_3	0.56	0.201	0.446

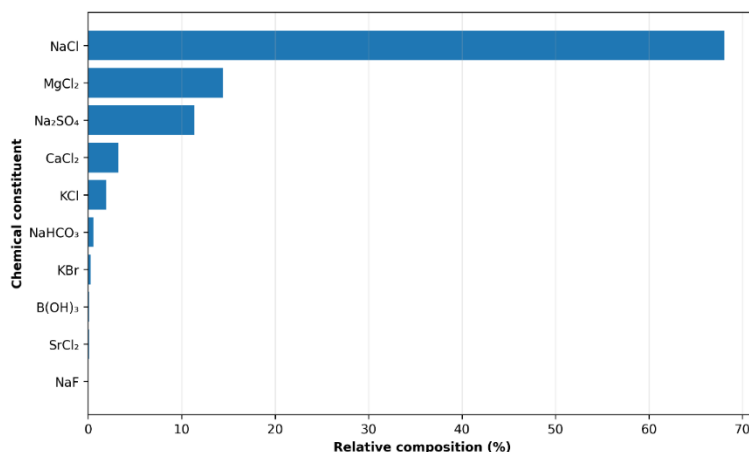


Figure 2. Relative Distribution of Major Constituents in High-Salinity Artificial Seawater

3.3 Concentration Scaling with Increasing Salinity

The proportionate increase in all the major constituents studied was observed over the range of salinity investigated.

Table 3 shows that NaCl increased by 29.941 g/L between 36,032 and 80,000 ppm, while MgCl₂ and Na₂SO₄ increased by 6.349 and 4.984 g/L, respectively. Concentrations of the major salts increased by ~2.22 fold at the highest TDS level.

The response to the target TDS and the total chemical concentration is shown in Fig. 3, which illustrates a good systematic concentration gradient but with the same formulation ratio.

Table 3. Concentration Changes Across the Artificial Seawater Salinity Gradient

Constituent	36,032 ppm (g/L)	80,000 ppm (g/L)	Increase (g/L)	Fold Change
NaCl	24.540	54.481	29.941	2.22
MgCl ₂	5.200	11.549	6.349	2.22
Na ₂ SO ₄	4.100	9.084	4.984	2.22
CaCl ₂	1.160	2.576	1.416	2.22
KCl	0.695	1.544	0.849	2.22

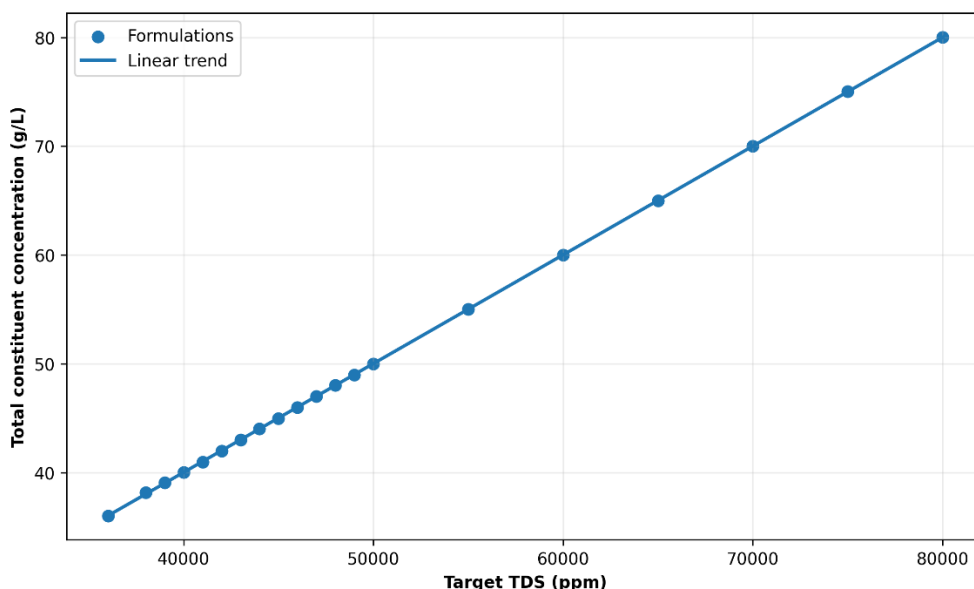


Figure 3. Relationship Between Target TDS and Total Chemical Concentration of Artificial Seawater

4.DISCUSSION

The results show a very well organized composition–salinity relationship of the artificial seawater formulations. An increase in total dissolved solids (TDS) (from 36,032 to 80,000 ppm) resulted in systematic increase in the level of all salts; however, the relative ratio of each other was maintained. NaCl was still the major component, accounting for about 68% of total composition, with MgCl₂ and Na₂SO₄ in the second and third, respectively. This trend suggests that the salinity gradient studied is more a proportional enrichment than a real change in the ionic matrix. The composition–property frameworks have also been employed to establish the relationships between the measurable material properties and the controlled compositional variation but in very different material systems (Minussi et al., 2024; Ren et al., 2023).

The predominance of NaCl has special significance in view of the physico-chemical behavior to be expected in concentrated system of electrolytes. All the factors of ionic concentration, charge, mobility and interactions between

dissolved species contribute to the electrical properties. Shcherbakov et al. (2021) showed that there are close relationships between the ion solvation, the dielectric behaviour and the electrical conductivity of electrolyte solutions. Similarly, Nau-Hix et al., (2021) found that the electrical conductivity and ionic composition can significantly affect the functioning of aqueous treatment systems. The highly proportional increase in NaCl, MgCl₂, Na₂SO₄, CaCl₂ and KCl here is therefore a good compositional starting point for further conductivity studies under high salinity conditions.

As dissolved-solute concentrations increase, osmotic behaviour is also likely to play a greater role. The ratio of major constituents concentrations between the lowest and highest TDS formulations is approximately 2.22 indicating a significant change in the solute environment. Marked physicochemical and biological response can occur under high osmolarity, for instance the metabolic behaviour of *Bacillus methanolicus* was found to be different for higher osmolarity by Frank et al. (2021). Although this biological system is quite different from artificial seawater, it is a good model for the functional role of osmotic conditions. It would thus be necessary to perform direct osmolality measurements to see if the proportional increase in salt concentration reported here is accompanied by a proportional increase in osmotic response or deviations due to non-ideal behaviour of concentrated solutions.

Another important aspect of seawater chemistry is the pH, as relatively small changes can affect chemical equilibria in seawater and chemical processes at marine interfaces. Orozco-Cruz et al. (2023) demonstrated the influence of the pH of seawater on the formation of calcareous deposits and cathodic protection behaviour. Biological systems can also be very sensitive to the decrease of seawater pH, as shown for the planktonic foraminifera by Dong et al. (2022). The results highlight the importance of adding pH as a parameter to describe artificial seawater in addition to salinity and ionic composition. However, measured pH values are not included in the present compositional data set, so that direct relationships between individual constituents and pH cannot be derived from the measured data.

A strong correlation between the target TDS and the total concentration of the constituents also further demonstrates the controlled nature of the formulation series studied. The relative proportions of ions stayed essentially the same, and the data should be useful in differentiating between the effects of concentration and changes due to major formulation changes. Concurrently measured pH, conductivity and osmolality data might be analysed by correlation, principal component analysis and multivariable modelling in the future. Multivariate methods prove especially useful when numerous environmental factors that are interrelated need to be analysed at the same time, as highlighted in water-quality assessment by Samraoui et al. (2024) and in analysing complex dynamic relationships by Abdollahi et al. (2025). More generally, multivariate optimization methods offer frameworks to assess different and related aspects of a complex system (Al Janabi, 2021).

The wide, systematically controlled salinity range and the extensive information obtained for 10 chemical constituents is thus the major asset of the analysis. Keeping the relative composition nearly constant decreases the variability in the ratio of the components' composition, and allows a clear characterization of concentration scaling. A potential downside to this is that the dataset available is for TDS and chemical composition, and not for measured chemical composition–property relationships of pH, conductivity, and osmolality. These physicochemical measurements could also be used in the future for direct experiment testing of nonlinear responses, ionic interactions, and multivariate predictors. The integration would be advantageous for the high salt content artificial seawater, as it would offer a better mechanistic understanding and increase its reproducibility for marine, electrochemical, desalination and controlled laboratory uses.

5.CONCLUSION

The analysis revealed a compositional gradient that was systematic over the different formulations of high salinity artificial seawater ranging from 36,032ppm to 80,000ppm TDS. The relative composition of the major chemical constituents remained fairly constant and the concentrations were increased in proportion to the increase in salinity. NaCl was predominant at around 68% and the five major salts accounted for ~99% of the formulation. The concentrations of major constituents rose by about an order of magnitude between the lowest and highest salinity conditions, and showed good agreement with the total chemical concentration and target TDS. These results show that the formulation series offers a controlled framework for the exploration of concentration-dependent behaviour with relatively little variation in the proportions of the salts. But, the data available will only support a conclusion as to salinity and chemical composition and not as to measured pH, conductivity or osmolality. Future studies using these physicochemical measurements would allow for direct measurement of the ionic interactions, the nonlinear responses, and the composition–property relations strengthening the applicability of the artificial seawater models in desalination, marine, and electrochemical studies.

REFERENCES

1. Abdollahi, S., Moradi, H., Pourmanafi, S., Modarres, R., & Fakheran, S. (2025). Multivariate analysis of dynamic correlations between urban form and air pollution: Implications for sustainable urban planning. *Sustainable Cities and Society*, 106637.
2. Al Janabi, M. A. (2021). Multivariate portfolio optimization under illiquid market prospects: a review of theoretical algorithms and practical techniques for liquidity risk management. *Journal of modelling in management*, 16(1), 288-309.
3. Berska, J., Bugajska, J., & Sztelfko, K. (2023). The accuracy of serum osmolality calculation in small children. *Journal of Medical Biochemistry*, 42(1), 67.
4. Büyükkaragöz, B., & Bakkaloğlu, S. A. (2023). Serum osmolality and hyperosmolar states. *Pediatric Nephrology*, 38(4), 1013-1025.
5. Dharmapriya, T. N., Rathnayake, I. M. S. K., Deeyamulla, M. P., Liyandeniya, A. B., Madhushani, L. S., & Priyantha, N. (2023). Comparison of ionic concentrations (Na^+ , Ca^{2+} , Mg^{2+} , NH_4^+ , Cl^- , SO_4^{2-} , NO_3^-) and water quality parameters of bulk depositions among three sites in Kandy area, Sri Lanka.
6. Dong, S., Lei, Y., Bi, H., Xu, K., Li, T., & Jian, Z. (2022). Biological response of Planktic foraminifera to decline in seawater pH. *Biology*, 11(1), 98.
7. Frank, C., Hoffmann, T., Zelder, O., Felle, M. F., & Bremer, E. (2021). Enhanced glutamate synthesis and export by the thermotolerant emerging industrial workhorse *Bacillus methanolicus* in response to high osmolality. *Frontiers in Microbiology*, 12, 640980.
8. Guo, L., Xie, Y., Sun, W., Xu, Y., & Sun, Y. (2023). Research progress of high-salinity wastewater treatment technology. *Water*, 15(4), 684.
9. Hasnain, M., Zainab, R., Ali, F., & Abideen, Z. (2025). An overview of biosorption, remediation, and desalination potential of algae to remove wastewater toxic pollutants for environmental safety. *Environmental Monitoring and Assessment*, 197(8), 853.
10. Henderson, M. A., Gillon, S., & Al-Haddad, M. (2021). Organization and composition of body fluids. *Anaesthesia & Intensive Care Medicine*, 22(8), 511-517.
11. Li, Z., Mao, C., Zhang, J., Hou, T., Zhang, Z., Zhang, K., ... & Yang, Z. (2025). Advances in Research on Desalination Technology for High-Sodium Wastewater. *Sustainability*, 17(1), 333.
12. Ligorì, N., Rajendiran, T., Prasad, M. M., & Vijayan, V. (2025). Assessment of groundwater vulnerability to seawater intrusion using GALDIT index in Chengalpattu District, Tamil Nadu. *Discover Geoscience*, 3(1), 250.

13. Minussi, F. B., Silva Jr, R. M., & Araújo, E. B. (2024). Composition-Property Relations for $\text{GAXFAyMA}_{1-x-y}\text{PbI}_3$ Perovskites. *Small*, 20(7), 2305054.
14. Najem, O., Shah, M. M., Zubair, M., & De Jesus, O. (2024). Serum osmolality. In StatPearls [Internet]. StatPearls Publishing.
15. Nau-Hix, C., Holsen, T. M., & Thagard, S. M. (2021). Influence of solution electrical conductivity and ionic composition on the performance of a gas-liquid pulsed spark discharge reactor for water treatment. *Journal of Applied Physics*, 130(12).
16. OGUNTADE, A. S. (2023). Hydrochemical and bacteriological evaluation of surface water and groundwater sources in Mpape Area of Abuja, North-Central Nigeria (Doctoral dissertation).
17. Omerspahic, M., Al-Jabri, H., Siddiqui, S. A., & Saadaoui, I. (2022). Characteristics of desalination brine and its impacts on marine chemistry and health, with emphasis on the Persian/Arabian gulf: a review. *Frontiers in Marine Science*, 9, 845113.
18. Orozco-Cruz, R., Bohórquez-Rico, J., Marin, D., Almeraya-Calderón, F., Espinoza-Vázquez, A., Carmona-Hernández, A., & Galván-Martínez, R. (2023). Effect of seawater pH variation on the growth of calcareous deposits and its effect on an impressed current cathodic protection system. *Journal of Solid State Electrochemistry*, 27(11), 3003-3016.
19. Ren, D., Wang, C., Wei, X., Lai, Q., & Xu, W. (2023). Building a quantitative composition-microstructure-property relationship of dual-phase steels via multimodal data mining. *Acta materialia*, 252, 118954.
20. Samraoui, K. R., Chelaghmia, M. L., & Samraoui, B. (2024). Multivariate analysis of water quality in the Seybouse River: implications for pollution management. *Environmental Quality Management*, 34(2), e22342.
21. Shcherbakov, V. V., Artemkina, Y. M., Akimova, I. A., & Artemkina, I. M. (2021). Dielectric characteristics, electrical conductivity and solvation of ions in electrolyte solutions. *Materials*, 14(19), 5617.
22. Vedaprakash, L., Senthilkumar, P., Inbakandan, D., & Venkatesan, R. (2022). Marine biofouling and corrosion on long-term behavior of marine structures. In *A Treatise on Corrosion Science, Engineering and Technology* (pp. 447-466). Singapore: Springer Nature Singapore.
23. Wang, J., & Huo, E. (2022). Opportunities and challenges of seawater desalination technology. *Frontiers in Energy Research*, 10, 960537.
24. Zavitsas, A. A. (2022). Properties of aqueous solutions. A treatise against osmotic and activity coefficients. *Journal of Molecular Liquids*, 348, 118410.