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INTEGRATION OF FLOW MODELLING, GEOCHEMISTRY AND ISOTOPIC TRACERS FOR SUSTAINABLE MANAGEMENT OF GROUNDWATER IN SIWA OASIS, WESTERN DESERT, EGYPT

Ph.D. Thesis Booklet

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1. Introduction

The global water crisis, characterized by diminishing water supply and quality, is particularly severe in arid regions like Egypt, posing a significant threat to agriculture and food security. In groundwater-dependent ecosystems such as the Siwa Oasis, sustainable management of water and soil resources is critical to maintaining the delicate water-salt balance, especially under the pressures of human development and climate change. The Siwa Oasis, entirely reliant on groundwater, faces pressing challenges, including waterlogging, soil salinization, and the deterioration of water quality. This research addresses these challenges through an integrated approach that combines advanced hydrogeological modeling, geochemical analysis, and isotopic tracing to develop a scientific basis for the sustainable management of the Oasis's vital groundwater resources.

2. Problem Statement and Research Aim

Siwa Oasis faces a severe water crisis due to unsustainable water management, leading to waterlogging, soil salinization, and declining water quality in the Tertiary Carbonate Aquifer (TCA). The current research aim to: 1) developing a high-resolution 3D hydrogeological model to characterize the subsurface architecture and fault systems; 2) diagnosing the drivers of soil salinization by quantifying the spatio-temporal dynamics of land use change, lake expansion, and soil salinization; 3) identifying groundwater recharge and salinity sources; 4) estimating residence time and recharge location to quantify inter-aquifer recharge and its structural controls; 5) developing a numerical flow model to predict the long-term impacts of groundwater abstraction; 6) assessing water quality and health risks from toxic elements; and 7) proposing a sustainable desalination solution by developing and evaluating an innovative, low-cost desalination technology.

3. Study Area Description

Siwa Oasis is an isolated closed depression located in the northwestern desert of Egypt (**Fig 1**). It is surrounded by the Mediterranean Sea to the north (approximately 330 km away), the Libya-Egypt border to the west (70 km), and Cairo to the east (560 km). The depression lies between latitudes 29.12°N and longitudes 25.43°E. Its total area is about 1,050 km and the population was approximately 23,546 residents.

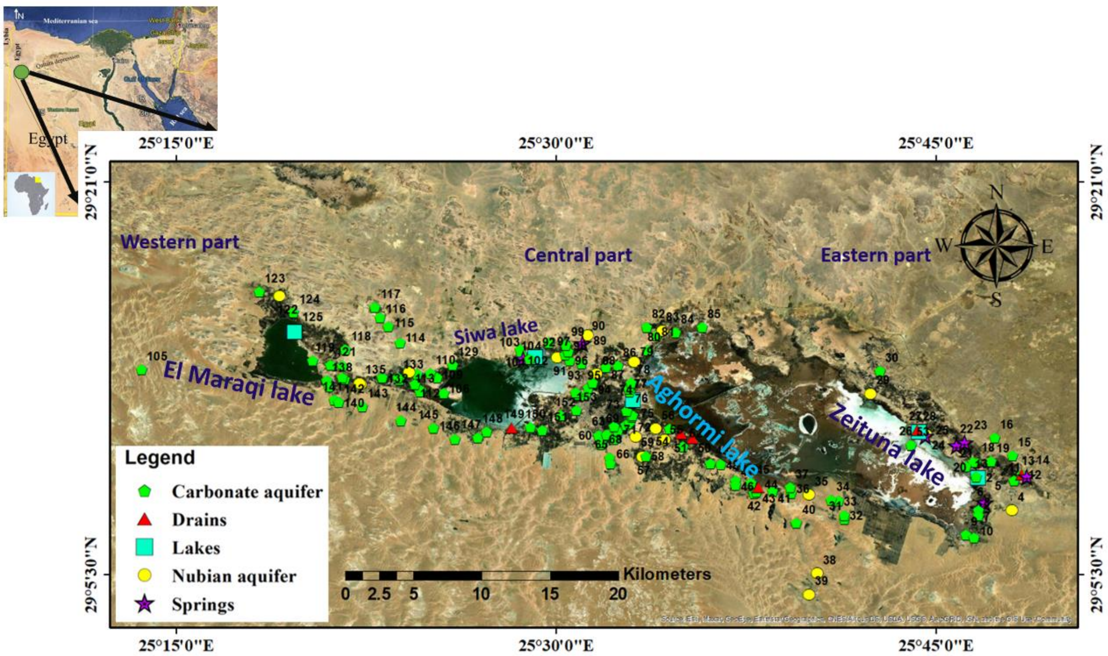

Figure 1. Location map and regional scale of the aquifer systems in Egypt

3.1. Water Resources and hydrogeology

Siwa Oasis relies heavily on both surface water and groundwater resources. Historically, the presence of four major lakes attracted settlers to the area. However, increasing salinity caused by high evaporation rates and agricultural drainage has rendered these lakes unsuitable for domestic use. The hydrogeology of Siwa Oasis is dominated by two main aquifer systems: the deep NSSA and the shallower TCA. These aquifers are part of a thick sedimentary sequence (approximately 3400 m) that ranges in age from the Paleozoic to the Recent. The cross section of the aquifer systems (**Fig 2**) from west to east showed that NSSA consists of multi layers affected by fault system and isolated from the TCA by aquiclude layer (upper cretaceous shale) modified after Elsheikh. The geological structure of the Oasis is complex, with a network of normal faults trending in N-S, E-W, NE-SW, and NW-SE directions. These faults play a critical role in controlling the lithofacies variations, the thickness of the geological formations, and the occurrence of natural springs. In the Siwa Oasis, the NSSA is the primary source of fresh water, with a total dissolved solids (TDS) content of less than 256 mg/l. The aquifer is composed of sandstone with intercalations of shale and clay. The water in the NSSA is over pressure (artesian). The groundwater flow from the south east and south west to the north and central Siwa Oasis (**Fig 2**). The TCA overlies the NSSA and is the primary source of water for irrigation in the Siwa Oasis. It is a semi-confined aquifer composed of Eocene-Miocene limestone and dolomite, with intercalations of shale, siltstone, sandstone, and evaporite deposits. The average thickness of the TCA is approximately 550 m.

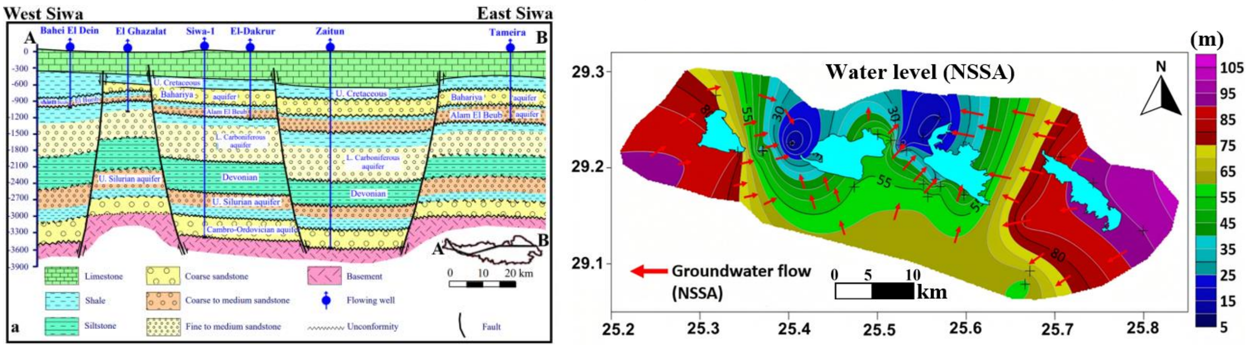

Figure 2. East-west cross section of the subsurface geology and groundwater flow direction

4. Material and Methods

To determine all the challenges in Siwa Oasis regarding water quality and quantity and find optimum solutions for these challenges, integrated approaches were applied with different materials and datasets as follow (**Fig 3**):

A) understand the aquifer systems from the geological and hydrogeological point of view to determine the lithofacies, aquifer and aquitard layers, heterogeneity, and build the geometry of the aquifers system. To achieve this, well logs including GR, SP, R, and lithological logs were used as well as applying two types of cluster analysis (K-means and SOM) to predict the lithofacies for the wells that lack the lithological logs

B) To determine the fracture and fault system that control the groundwater flow and location where different water resources could mix between different aquifers and surface water, aeromagnetic data with edge filtering were used and validated with 2D and 3D inversion and well logs correlation.

C) To determine petrophysical and hydraulic parameters that are very important factors needed in the Numerical flow model, pumping test data and well logs data were used based on cooper Jacob and Kozeny Karmen methods.

D) The remote sensing data and SVM were used to detect the changes in the surface area of the salt lakes and water logging in the soil that increased the soil salinization and reduced plant production.

E) The physicochemical parameters, heavy metal, stable isotopes, and radiocarbon were used for several aims including 1) type of salts and minerals could accumulate in the soil using PHREEQC geochemical model, 2) determine the recharge source, salinity origin, residence time, and mechanism controlling water chemistry in the aquifer system based on different mixing models, 3) The suitability of water resources for drinking purposes and health risk of toxic metals using ANN and Monte Carlo simulation.

F) Integration of multiple data and results from previous findings of using well logs, aeromagnetic data, pumping test, remote sensing, stable isotopes and radiocarbon to build numerical flow model and estimate the sustainability of the groundwater in the aquifer systems and predict the future risk from drawdown in the water level. The model also aimed to validate the findings of the multi-isotopic data regarding groundwater salinization and recharge source.

G) Examination of innovative solution to decrease groundwater and soil salinization using raw material such as Diatomite and Kaolinite to create effective Zeolite geopolymer in salt rejection.

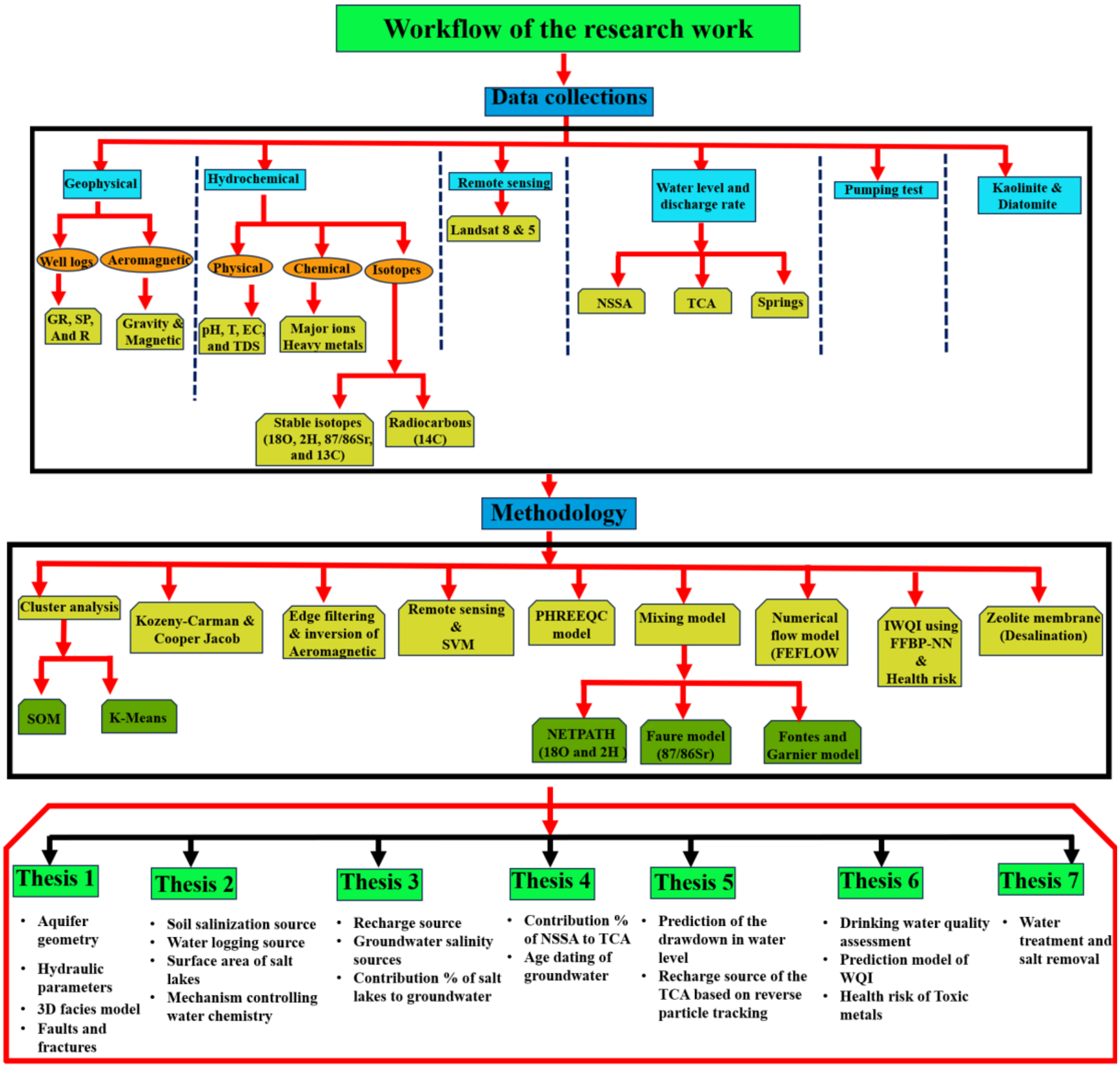

Figure 3. The research framework showing the datasets used, methodology, and results

5. Results and Discussion

The research yielded significant new insights into the hydrogeology of the Siwa Oasis, providing a comprehensive understanding of the aquifer system, the drivers of environmental degradation, and potential solutions for sustainable water management. Following the established workflow for the application of the above-exposed methods on the constructed database of Siwa Oasis, the new scientific results could be summarized in 7 theses as follows;

5.1. Aquifer Characterization and Structure Controlling Aquifer System

This thesis establishes and validates a novel, cost-effective workflow for the detailed characterization of complex, multi-layered aquifer systems in data-scarce arid regions. By integrating advanced machine learning with traditional geophysical and hydrogeological data, this study provides an unprecedentedly clear and quantitative 3D visualization of the subsurface architecture of the Siwa Oasis. The primary scientific contribution is the successful application of an integrated workflow that synergizes Self-Organizing Maps (SOM) and K-means clustering of well-log data (GR, SP, Resistivity) to classify the subsurface hydrostratigraphic facies. This data-driven approach provides a robust and cost-effective alternative to traditional, expensive cutting sample analysis. The resulting classification was then used to construct a high-resolution 3D geological model, visualizing the spatial distribution and continuity of the key aquifer (sandstone facies) and aquitard (shale facies) layers. Furthermore, this study presents a significant methodological advance by integrating high-resolution aeromagnetic and gravity data to map the deep structural framework controlling the aquifer system. By integrating this structural map with the 3D geological model, this work provides a comprehensive understanding of the specific pathways governing groundwater flow and hydraulic connectivity between the deep NSSA and the shallow TCA. The main key findings of thesis 1 could be concluded as follows;

1. Self-Organizing Maps (SOM) and k-means clustering successfully delineated three distinct lithological units within the NSSA (sand layers, shaly sand, and shale) with SOM proving more accurate than k-means for estimating aquifer layer thickness and providing higher-resolution identification of thin layers. This method could be applied incase lack of data from cutting samples or lithological logs (**Fig 4**).

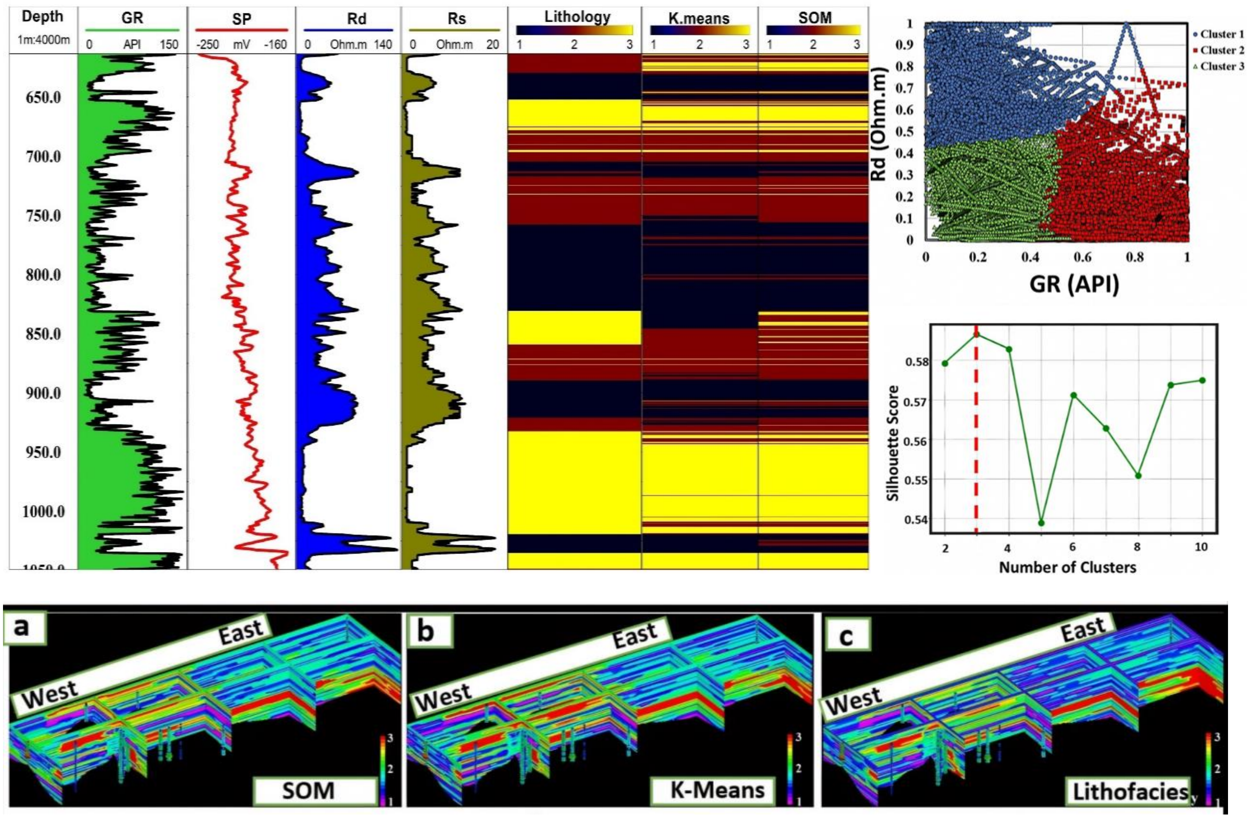

Figure 4. (a) Visualization of the well logs in Sharqia borehole in 1D with two types of clusters validated with lithological log with relationship between resistivity and GR for all wells and silhouette score. Fence diagram demonstrates the interpolation of SOM clusters (a), k-means clusters (b) and lithology (c) in 3D showing the heterogeneity of the NSSA with upper cretaceous shale.

2. Hydraulic conductivity validation using both Kozeny-Carman (**Fig 5**) and Cooper-Jacob methods showed strong agreement ($R^2 = 0.92$), with the highest values in central Siwa Oasis. The hydraulic conductivity ranged from 1.2 m/d to 6.6 m/d and effective porosity from 0.2 to 0.3 which could be used for groundwater flow modeling.

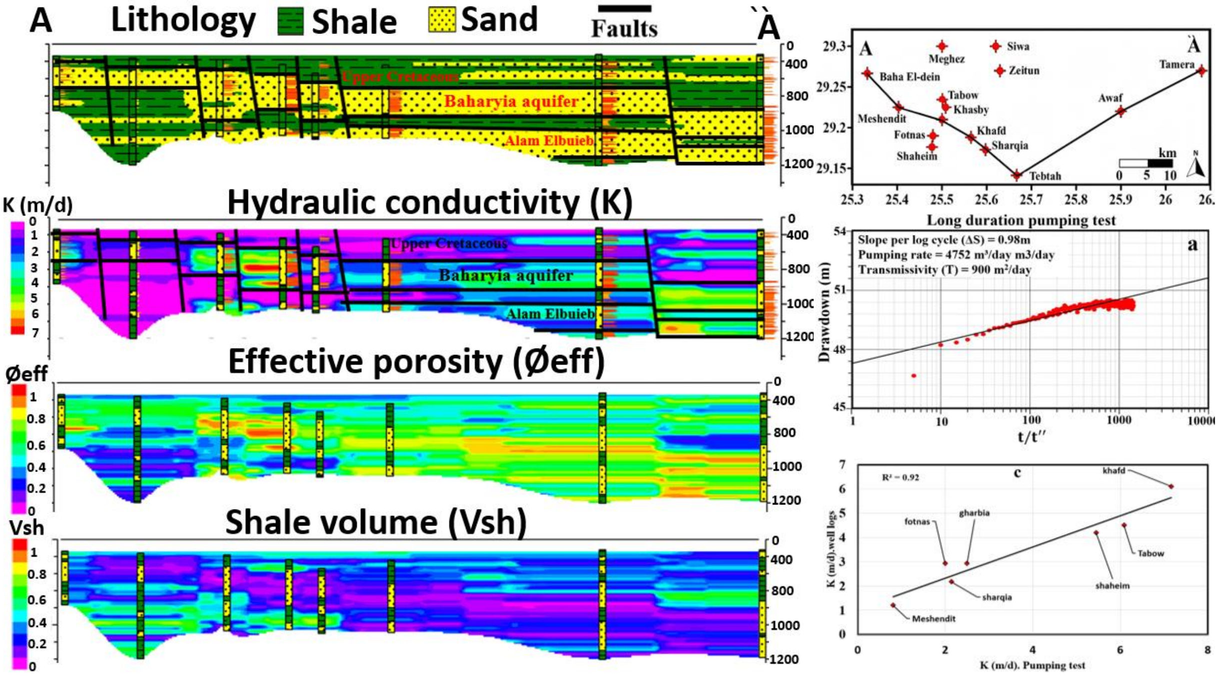

Figure 5. Interpolation of the lithology, hydraulic conductivity, effective porosity, and shale volume in 2D showing the hydrostratigraphic units and fault plane along A-À cross section and relationship between drawdown and time for long duration pumping test (a) calibration curve of hydraulic conductivity estimated from well logs vs pumping test (c)

3. Integrated gravity and magnetic data analysis (**Fig 6**) identified dominant NE-SW, NW-SE, and E-W lineament trends that control groundwater flow dynamics, with fractures in the shallow carbonate aquifer acting as pathways for surface water leakage and faults in the NSSA serving as conduits for upward flow to recharge TCA.

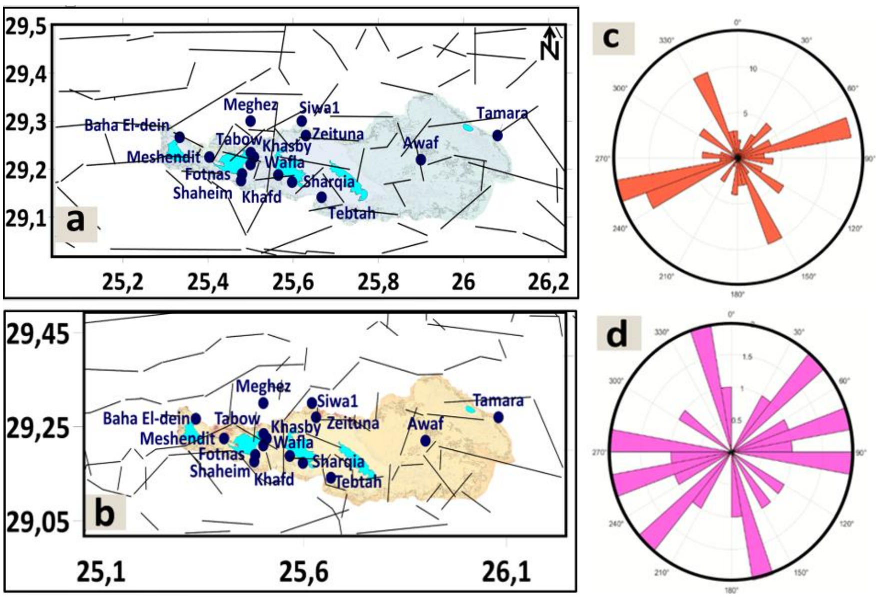

Figure 6. Combined Lineament map of the gravity and magnetic from different edge filtering techniques with 0.5km (a), 3.5km (b), and the resultant rose diagram showing predominantly NE-SW, NW-SE and E-W trend (c, d)

4. 3D gravity inversion modeling revealed that basement depths ranging from 2.5 km to over 4.5 km and the TCA from 360 m to 630 m (**Fig 7**).

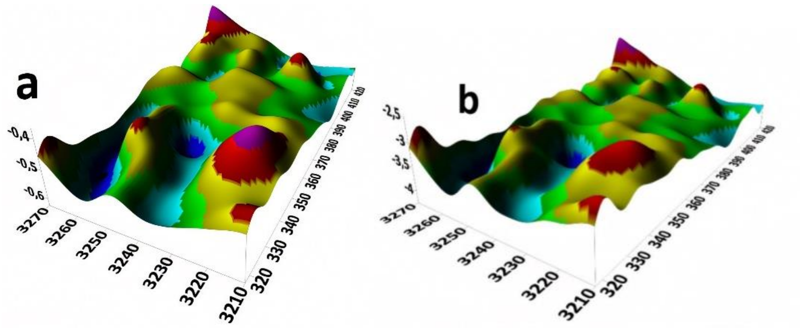

Figure 7. (a, b) 3D model of estimated depth, in the study area for the shallow TCA (a) and deep NSSA (top of the basement) (b)

5.2. Soil Salinization Origin and mechanism controlling water chemistry

This thesis provides a comprehensive diagnosis of the escalating soil salinization in Siwa Oasis by pioneering an integrated approach that combines multi-temporal remote sensing, machine learning, and detailed hydrogeochemical analysis. This thesis moves beyond simply identifying salinization to quantitatively linking it to specific land-use changes and elucidating the complex geochemical processes that govern water quality degradation.

The primary new scientific result is the quantitative, time-series evidence linking the expansion of agricultural land with the dramatic growth of hypersaline lakes and subsequent soil salinization. Over a 30-year period (1990-2020), cultivated land increased by 270%, which directly corresponds to a 168% increase in the surface area of salt lakes due to increased agricultural drainage. This study is the first to establish this direct quantitative relationship for Siwa Oasis. The key methodological advance was the application of a Support Vector Machine (SVM) classifier to a consistent set of Landsat imagery, which allowed for objective and repeatable land use/land cover mapping over three decades, a significant improvement over subjective, manual interpretation methods. The main key findings of thesis 2 are as follows;

1. Remote sensing analysis and SVM could predict the rapid increase of hypersaline lakes (**Fig 8**) from 22.6 km² in 1990 to 60.6 km² in 2020 causing soil salinization. Zeitun lake showed no significant increase in the surface area which could give indication of probability of leakage downward to the TCA through the fracture system and increase the groundwater salinization.
2. Hydrochemical evaluation revealed that the NSSA contains freshwater dominated with Mixed Ca-Mg-Cl-SO4, while the TCA and springs are brackish to saline, and lakes are hyper saline water dominated with Na-Cl and Ca-Mg-SO4 facies (**Fig 9**).
3. The main mechanism controlling water chemistry are calcite, dolomite, halite, gypsum dissolution, silicate weathering and ion exchange and evaporation.
4. Geochemical modeling (**Fig 10**) using PHREEQC identified mineral supersaturation conditions for montmorillonite, calcite, dolomite, and clay minerals that reduce soil permeability and increase waterlogging.

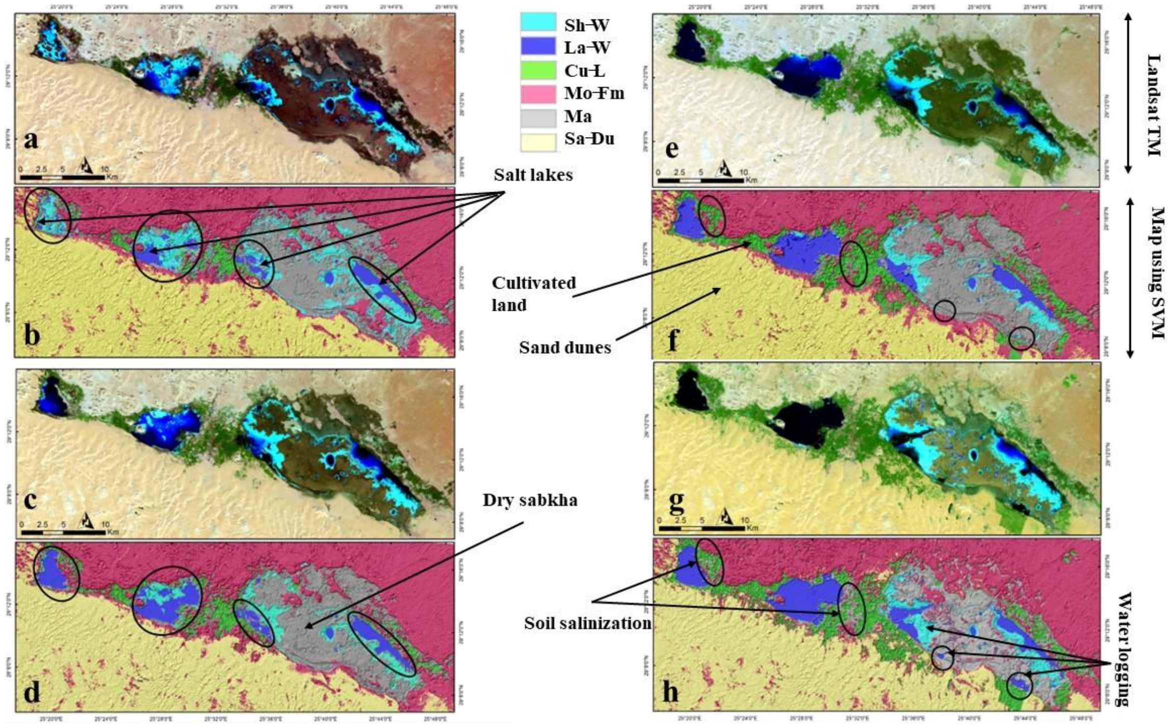

Figure 8. FCC 7-4-2 in RGB respectively for Landsat TM a) 1990, c) 2000, e) 2010, g) OLI 2020 and their corresponding resultant thematic map using SVM (b, d, f, and h respectively).

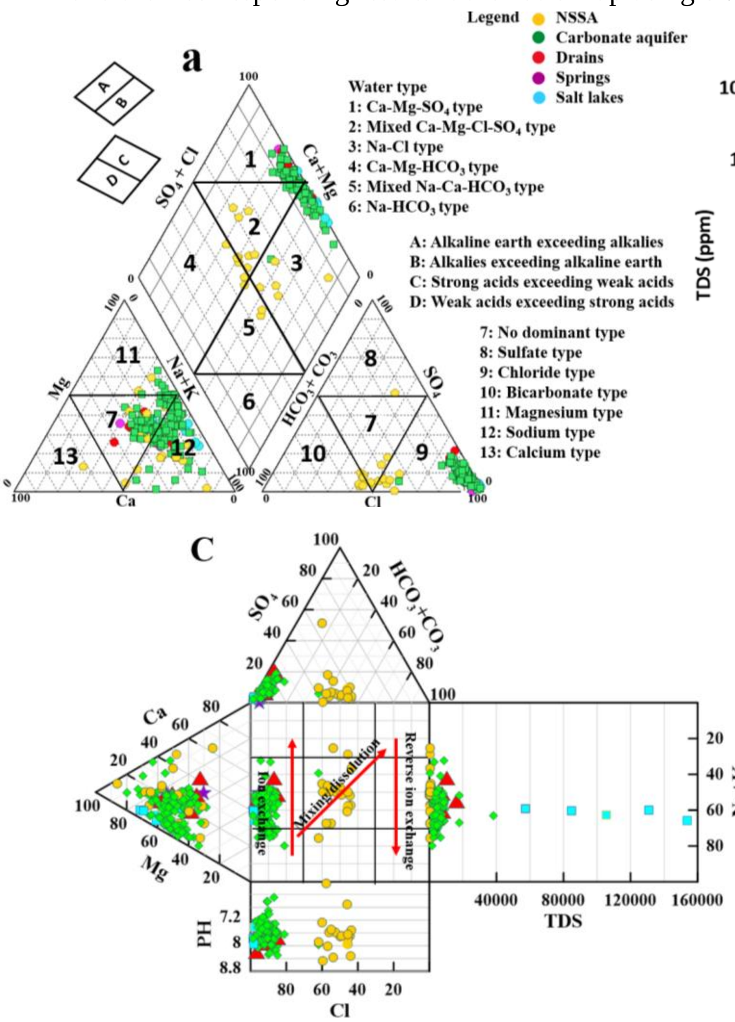

Figure 9. Graphical representation of Piper (a), Gibbs (b), and Durov (c) diagrams

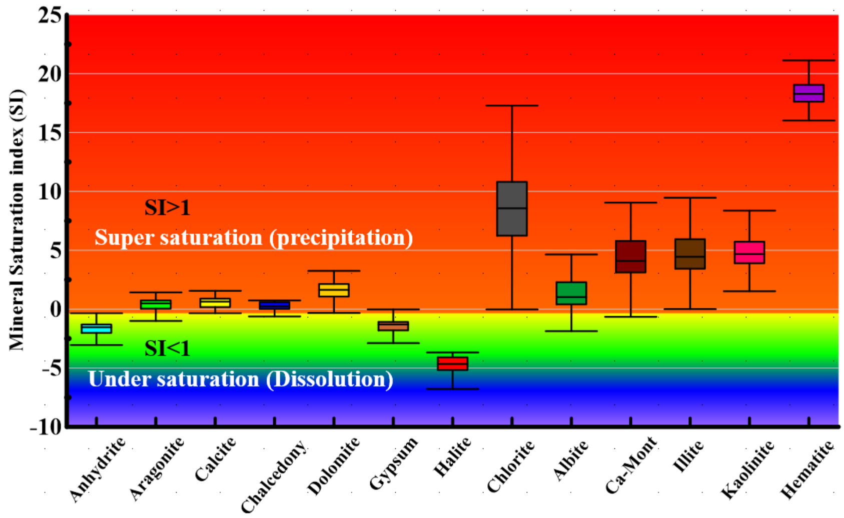

Figure 10. Minerals saturation index extracted from PHREEQC model.

5.3. Groundwater Recharge Source and Salinity Origin

This thesis provides a definitive identification of the recharge sources and salinity origins in the Siwa Oasis aquifer system by employing combination of stable isotope analysis (δ^2H, $\delta^{18}O$), advanced statistical techniques (PCA, K-means), and inverse NETPATH mixing models. This thesis moves beyond qualitative descriptions to deliver a quantitative assessment of the complex mixing processes that govern the oasis's water quality.

The primary new scientific result is the quantitative confirmation of a dual-source mixing model for the TCA. By using stable isotopes as tracers, this study proves that the TCA's water is a mixture of upward leakage from the fresh NSSA and downward intrusion from the hypersaline surface lakes. A key methodological advance was the use of PCA to reduce the dimensionality of the complex hydrochemical dataset, followed by K-means clustering to objectively group water samples into three distinct groups. This allowed for the precise selection of representative end-members (NSSA and Salt Lake water) and mixed samples (TCA water) for the mixing model, a significant improvement over subjective, manual selection. The model subsequently quantified the contribution of each source to the TCA's salinity, a critical new finding for management. The main key findings of thesis 3 are as follow;

1. Stable isotope analysis revealed that both the NSSA and TCA contain paleo-meteoric (**Fig 11**) water with $\delta^{18}O$ values ranging from -10.71 to -8.57‰ for NSSA and -10.62 to -8.45‰ for TCA, while salt lakes showed highly enriched values (-7.09 to -0.85‰) due to intense evaporation.
2. PCA identified four key components explaining 75.07% of total variance, with PC1 (40.5%) representing overall **mineralization and salinity**, PC2 (15%) indicating recharge sources and **evaporation effects**, PC3 (11.9%) reflecting trace metal concentrations from **geological formations**, and PC4 (7.64%) showing human-induced contamination from **agricultural activities.**
3. K-means clustering analysis successfully identified three distinct hydrochemical clusters with average electrical conductivity values of 7,000 µS/cm, 10,000 µS/cm, and 2,500 µS/cm, effectively distinguishing between different water sources and mixing processes affecting groundwater quality.
4. NETPATH mixing model (**Fig 12, table 1**) quantified that hypersaline lakes contribute 0.6-4% to TCA salinity through downward seepage with the highest contribution from Zeitun lake, while NSSA provides 63-87% freshwater contribution through upward flow, with strong model calibration (R^2 = 88%) confirming that despite small percentages, the extremely high TDS of salt lakes (130,992-153,589 mg/L) significantly impacts groundwater quality.

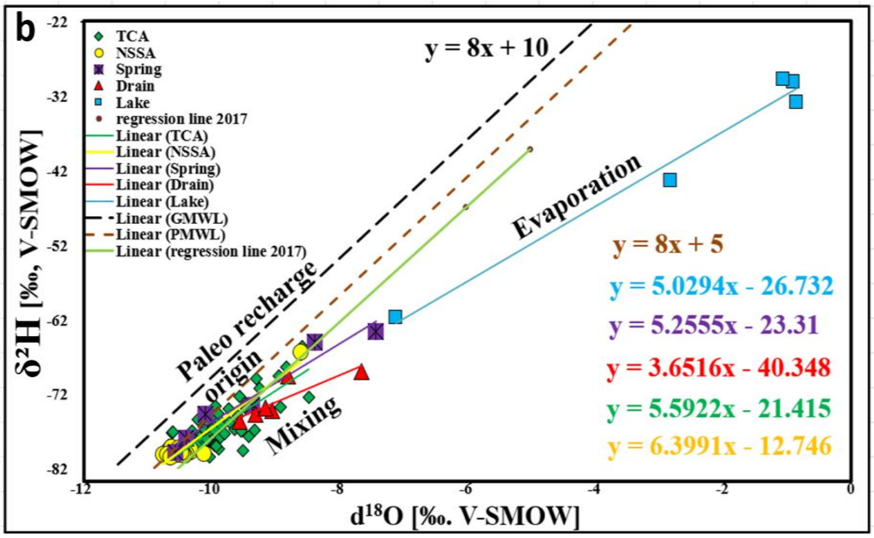

Figure 11. Plotting graph of δ^2H and $\delta^{18}O$

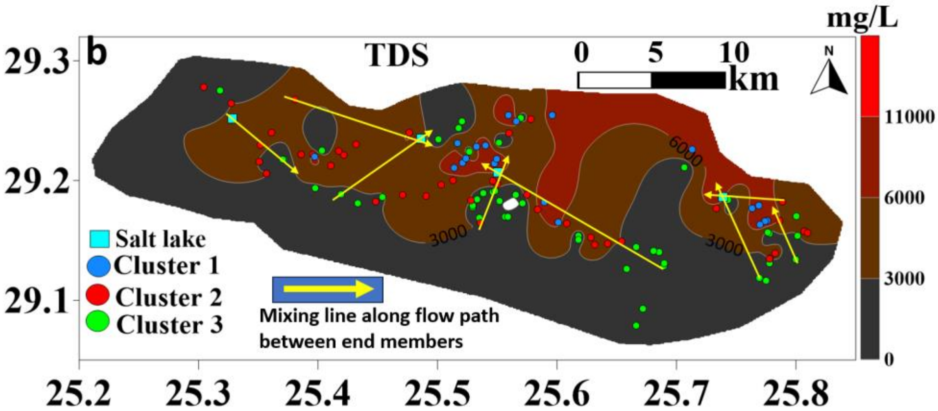

Figure 12. The distribution map of the TDS with the mixing line between the endmembers

Table 1. The seven models, including the two initial water, the final water from the cluster as well as the mixing percentage

Model number	Site	Model type	Initial 1	Initial 2	Final	Mixing % calculated		Mixing % computed	
						Initial 1	Initial 2	Initial 1	Initial 2
1	Zeitun	Reaction and mixing	9 (TCA, cluster 3)	27	20	0.84	0.16	0.97	0.02
2	Zeitun		10 (TCA, cluster 3)	27	21	0.82	0.18	0.99	0.009
3	Zeitun		7 (TCA, cluster2)	27	21	0.82	0.18	0.96	0.04
4	Siwa		144 (TCA, cluster3)	92	93	0.98	0.02	0.99	0.006
5	Siwa		117 (TCA, cluster2)	92	87	0.96	0.04	0.98	0.02
6	Zeitun		21 (TCA, cluster1)	4	15	0.26	0.74	0.13	0.87
7	Siwa		87 (TCA, cluster1)	56	68	0.14	0.86	0.37	0.63

Model number	Phase precipitated or dissolved									
	Calcite	Dolomite	Halite	Gypsum	Ca-Montmorillonite	Na-Montmorillonite	Chalcedony	Illite	Exchange	Ev
1	-1.2	0.8	41.7	-1.6	-	-1.2	-	1.2	1.2	1.04
2	-3.15	1.5	30.3	-	-0.72	-	0.03	0.73	-7.3	1.6
3	-	1.2	58.4	0.9	-	-4.38	1.87	4.4	-19.4	1.5
4	-	-0.48	38.4	-0.69	-	-0.6	0.01	0.6	-5.7	1.6
5	-15.3	7.2	0	-2.01	-	0.41	-0.15	-0.4	-10.8	1.4
6	3.29	-2.29	0	0.98	-	0.25	-0.17	-0.27	1.27	2.07
7	-	1.3	20.9	5.34	-	-1.42	2.21	1.44	-4.36	2.3

5.4. Residence Time Estimation and Recharge Location of the TCA from NSSA

This thesis provides a quantitative and spatially explicit understanding of the recharge dynamics and groundwater residence times in the Siwa Oasis aquifer system (**Fig 14**). By pioneering the combined application of multiple isotopic tracers (including δ^2H, $\delta^{18}O$, $^{87}Sr/^{86}Sr$, ^{13}C and ^{14}C) with a dual-model approach (Faure and NETPATH inverse mixing models), this thesis moves beyond qualitative inference to deliver precise, quantitative estimates of inter-aquifer recharge and its structural controls.

This work provides definitive confirmation for the long-held hypothesis that faults and fractures act as the primary conduits for vertical recharge from the NSSA to the TCA and leakage of salt lake's water to the shallow TCA and fractures. The main findings of this thesis are as follow;

1. Multi-isotopic tracer analysis using δ^2H, $\delta^{18}O$, ^{13}C, ^{14}C, and $^{87}Sr/^{86}Sr$ revealed distinct spatial patterns with NSSA showing uniform Sr concentrations (0.04-0.28 mg/L) and $^{87}Sr/^{86}Sr$ ratios ranging from 0.709-0.715, while TCA exhibited highly variable Sr concentrations (1.074-10.1 mg/L) with minimal $^{87}Sr/^{86}Sr$ variation (0.708-0.709), indicating different water-rock interaction processes.
2. The Faure mixing model successfully quantified NSSA contributions to TCA recharge, demonstrating 80-90% NSSA input in low-salinity areas (1000-2000 mg/L) along fault planes, 50-80% in intermediate zones (2000-5000 mg/L), and minimal contributions (0-40%) in high-salinity northern regions (5000-9000 mg/L) near salt lakes.
3. NETPATH inverse mixing model validation showed excellent agreement with the Faure model (R^2 = 0.96), confirming NSSA contributions ranging from ~90% in southeastern fault zones to ~52% in northern high-salinity areas, with geochemical processes including calcite/dolomite precipitation in NSSA-dominated regions and halite/gypsum dissolution in evaporative zones.
4. Groundwater age correction using radiocarbon dating revealed significant temporal variations with TCA ages ranging from 640-13,551 years and NSSA ages from 4,296-14,184 years, showing a clear spatial trend of decreasing age from southeast to north, with youngest ages near Siwa Lake indicating active mixing and recharge processes. The relationship between $^{87}Sr/^{86}Sr$ ratios and groundwater age demonstrated that older groundwater (>10,000 years) concentrated near fault systems preserves paleowater from the African Humid Period, while younger northern waters reflect mixing with surface sources (salt lakes), confirming that structural features control both recharge pathways and preservation of ancient groundwater signatures.
5. The findings also provide a generalizable insight for water management in multi-layered aquifer systems: protecting the integrity of deep, pristine aquifers requires not only managing direct abstraction but also understanding and managing the structural pathways that connect them to shallower, more vulnerable aquifers. This has significant implications for the placement of new wells and the development of sustainable abstraction strategies in arid regions globally.

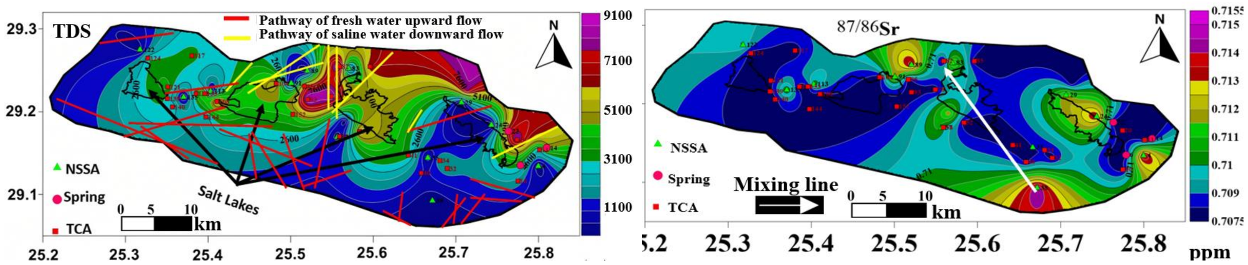

Figure 13. The distribution maps of the TDS and 87/86Sr in the study area

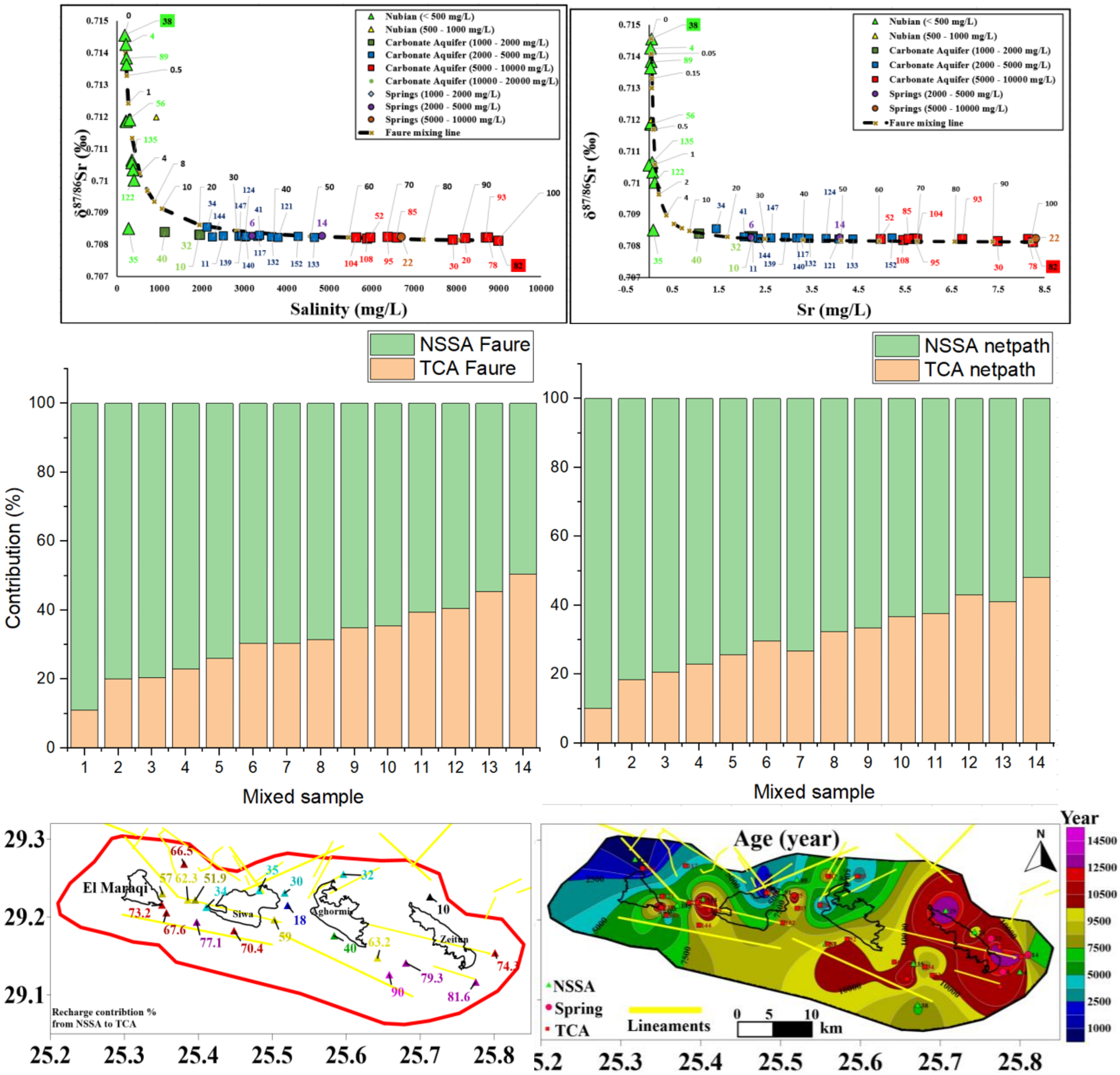

Figure 14. The relationship between salinity vs $^{87/86}$Sr and Sr vs $^{87/86}$Sr supported with mixing line based on Faure model and validation with NETPATH mixing model and distribution map of the contribution % from NSSA and corrected age of the groundwater in the aquifer systems

5.5. Numerical flow model using backward particle tracking

This research presents the first fully integrated, three-dimensional numerical flow model of the Siwa Oasis, providing a powerful tool for predicting the long-term impacts of groundwater abstraction and for validating the conceptual hydrogeological model (**Fig 15**). By coupling the NSSA and TCA and explicitly incorporating major fault and fracture systems, this model offers unprecedented predictive capabilities and a clear visualization of the complex flow dynamics. The key methodological advance was the use of reverse particle tracking to visually and quantitatively validate the recharge pathways inferred from the geochemical and isotopic data. This is the first model for Siwa Oasis to use this technique, providing direct visual evidence of upward leakage from the NSSA to the TCA along fault planes and, crucially, downward leakage from the surface salt lakes. The primary new scientific result is the quantitative prediction of a catastrophic hydraulic gradient reversal between the TCA and the NSSA within 150-200 years under current abstraction rates. This finding elevates the issue from a problem of water scarcity to a potential ecological and humanitarian crisis, as it would lead to the permanent contamination of the region's only freshwater source. The main key findings of this thesis are as follow;

1. Groundwater numerical flow modeling using FEFLOW demonstrated critical drawdown patterns from 1960-2025, showing dramatic water level decline from 175m to 75m above sea level in western areas and slower decline from 142m to 128m in eastern regions, with future predictions indicating water levels will drop to 30-70m by 2100 under current extraction rates of 330,000 m³/day (**Fig 16**).
2. Spring discharge monitoring showed significant decline from 3,900 m³/d in 1960 to 3,000 m³/d in 2025, with projections indicating further reduction to 2,400 m³/d by 2100, directly correlating with decreasing pressure heads and threatening natural water resources for agriculture and tourism.
3. Reverse particle tracking analysis provided definitive validation of NSSA to TCA recharge mechanisms, with all 24 particles released from each TCA tracing back to the NSSA along distinct fault and fracture pathways, confirming that structural features serve as primary conduits for upward groundwater flow between aquifer systems. The pathlines reaches the salt lakes confirming the leakage downward of salt lakes (**Fig 16**).
4. The modeling results identified a critical threshold scenario where NSSA may cease recharging TCA within 150-200 years under current extraction rates, potentially reversing flow dynamics and causing saline TCA water to contaminate the freshwater NSSA, representing an existential threat to Siwa Oasis's water security and requiring immediate sustainable management interventions (**Fig 16**).

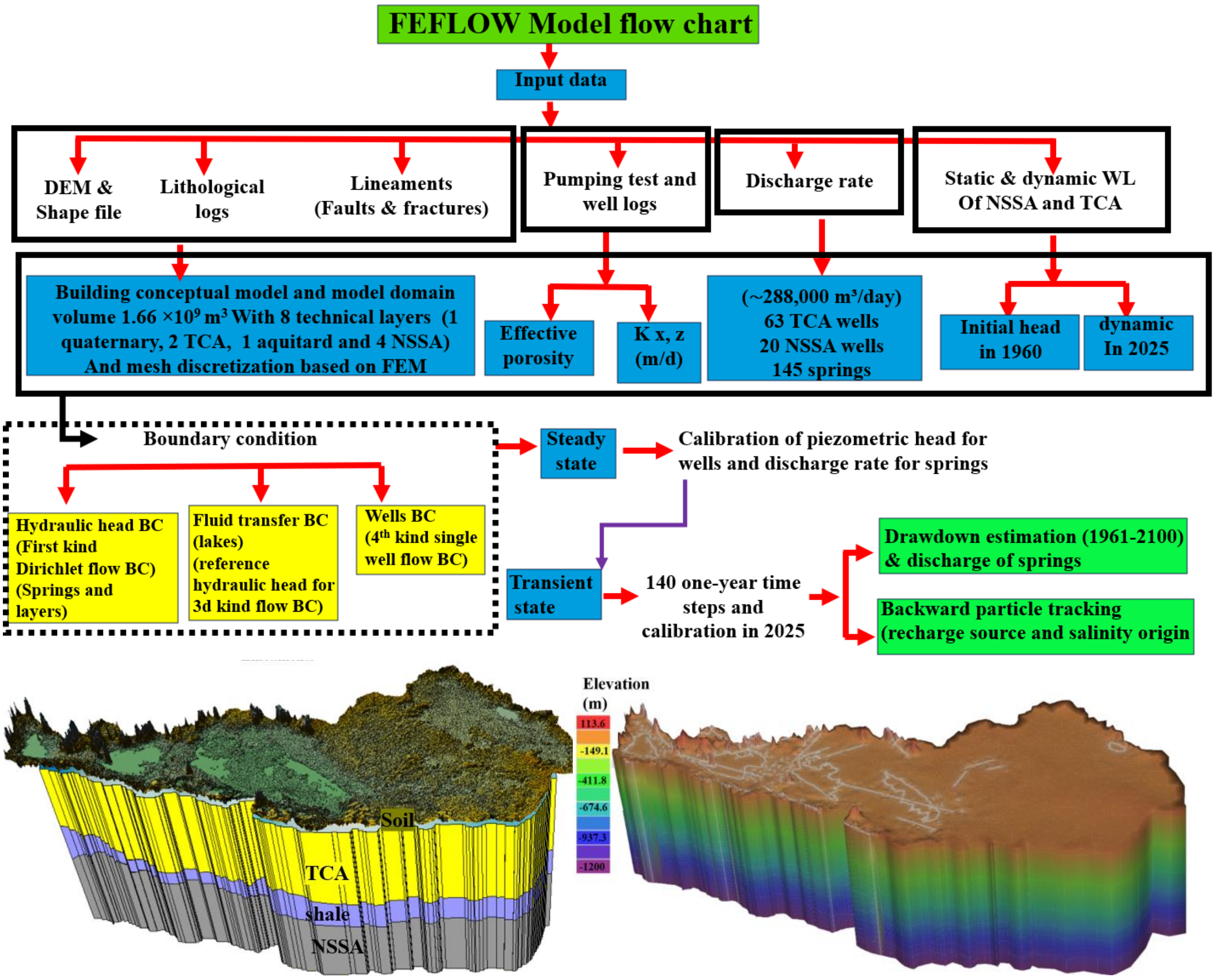

Figure 15. The frame work of used to build the numerical flow model and the model boundary including structure lineaments and lakes boundary, 3D geometry of the study area constructed based on well log correlations with 3D discretization using FEM

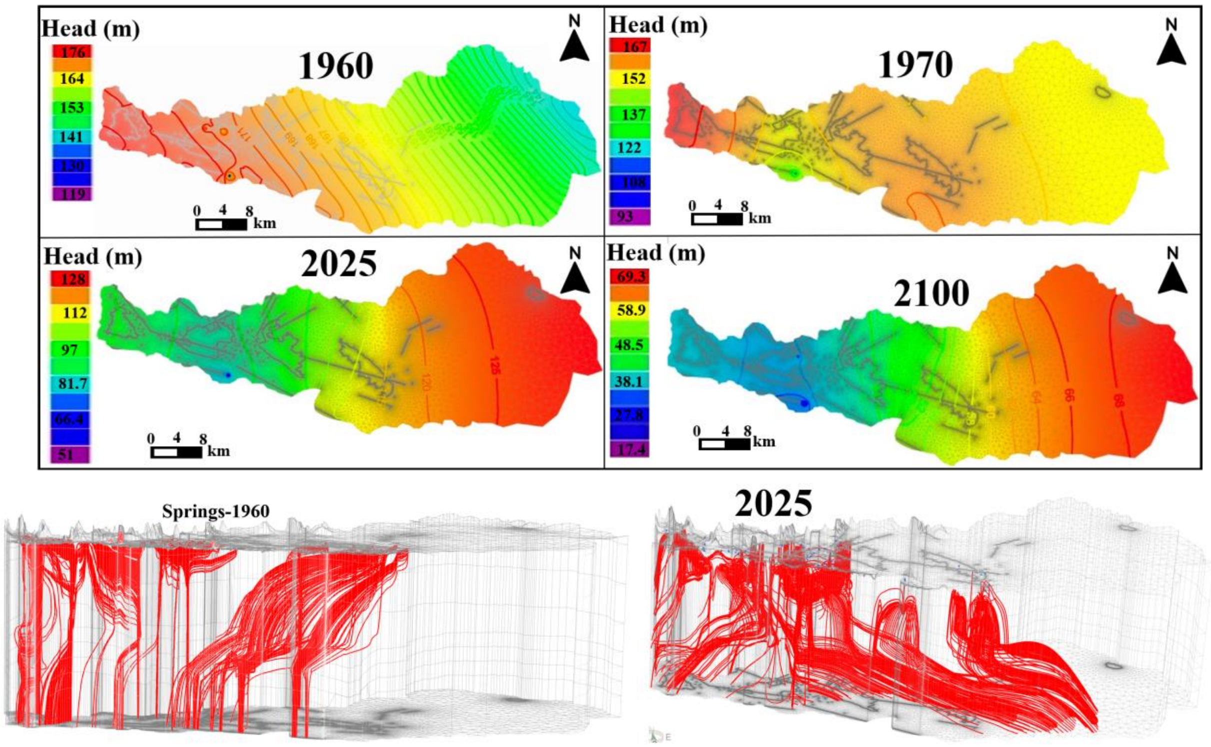

Figure 16. The changes in the water level in the NSSA from 1960 (initial head) to the current state (2025) and predicted water level in 2100. Reverse particle tracking from wells in 2D and 3D showing the recharge area in east of Siwa Oasis and recharge of TCA from NSSA through faults and fracture system based on the pathlines.

5.6. Water Quality and Health Risk Assessment of Potential Toxic Elements

This thesis pioneers a comprehensive framework for assessing the suitability of water resources for human consumption and quantifying the associated health risks in the Siwa Oasis. By integrating a novel Integrated Weighted Water Quality Index (IWQI) with advanced machine learning (FFBP-NN) and probabilistic risk assessment (Monte Carlo simulation), this study moves beyond deterministic water quality standards to provide a nuanced, risk-based evaluation of water safety.

The integrated water quality assessment based on the IWQI revealed a clear spatial distinction in groundwater quality across the Siwa Oasis aquifer system. Nearly half of the water samples were classified as extremely poor for drinking purposes, with the TCA showing widespread deterioration due to salinity increases from water–rock interactions, excessive groundwater abstraction, and return flow from agricultural drainage. In contrast, the deep NSSA generally contained good-quality fresh water, particularly toward the eastern part of the study area, where confined conditions provided protection from salinization and contamination. These findings underscore the vulnerability of the TCA to anthropogenic pressures and hydrogeological processes, while highlighting the relatively better preservation of water quality within the NSSA (**Fig 17**).

The application of the FFBP-NN prediction model demonstrated excellent performance, with regression coefficients consistently exceeding 0.95 across training, validation, and testing phases (**Fig 17**). The optimized model, relying on a reduced set of 12 parameters, was able to predict IWQI values with high accuracy and robustness, eliminating the need for exhaustive and costly measurements such as Ca^{2+} and Mg^{2+}. This confirms the model's capacity to capture the complex nonlinear relationships between hydrochemical variables and water quality indices. By accurately reproducing the observed IWQI distribution across both the NSSA and TCA, the model provided a reliable and cost-effective tool for large-scale water quality monitoring and management.

Overall, this study highlights two important outcomes: (i) the groundwater quality in Siwa Oasis is highly variable, with significant risks associated with over-exploitation and salinization of the TCA, and (ii) advanced machine learning approaches, such as FFBP-NN, offer powerful predictive capabilities that can complement traditional monitoring. These insights are crucial for guiding sustainable groundwater management strategies in arid regions, ensuring safe drinking water supplies while supporting agricultural productivity.

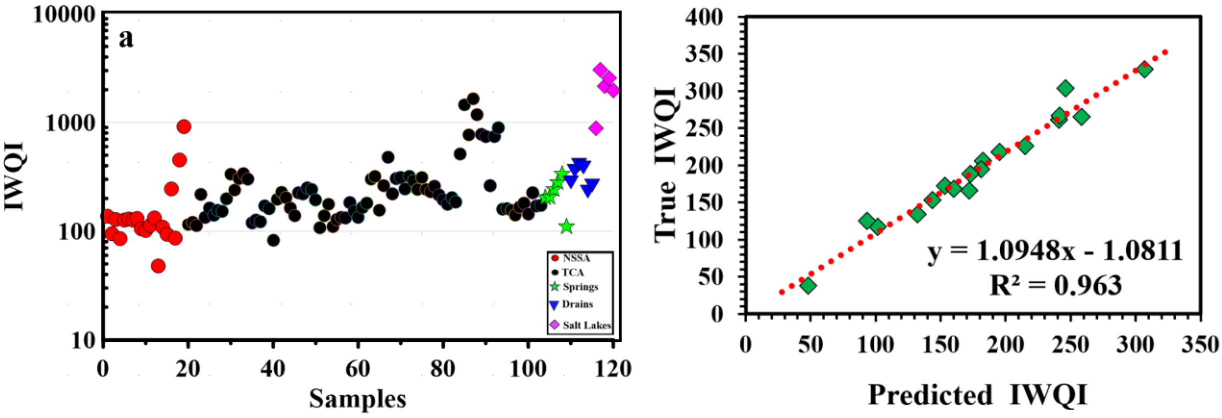

Figure 17. Ploting of samples with the values of IWQI (a) and the relationships between the true values and predicted values of the water quality (b)

The health risk assessment of toxic metals in Siwa Oasis groundwater highlights a serious threat to public health, particularly for children. Non-carcinogenic risk analysis (**Fig 18**) revealed that oral ingestion poses a far greater hazard than dermal exposure, with cadmium (Cd), chromium (Cr), and lead (Pb) consistently exceeding the safety threshold (HQ > 1) in most samples. Children were disproportionately affected, with more than 75% of sampling sites exceeding the acceptable hazard index (HI) for oral exposure, compared to adults who were less vulnerable but still at significant risk. Dermal exposure risks were generally low for adults but remained concerning for children, especially for Cd and Cr, underscoring the heightened vulnerability of younger populations to toxic metal contamination.

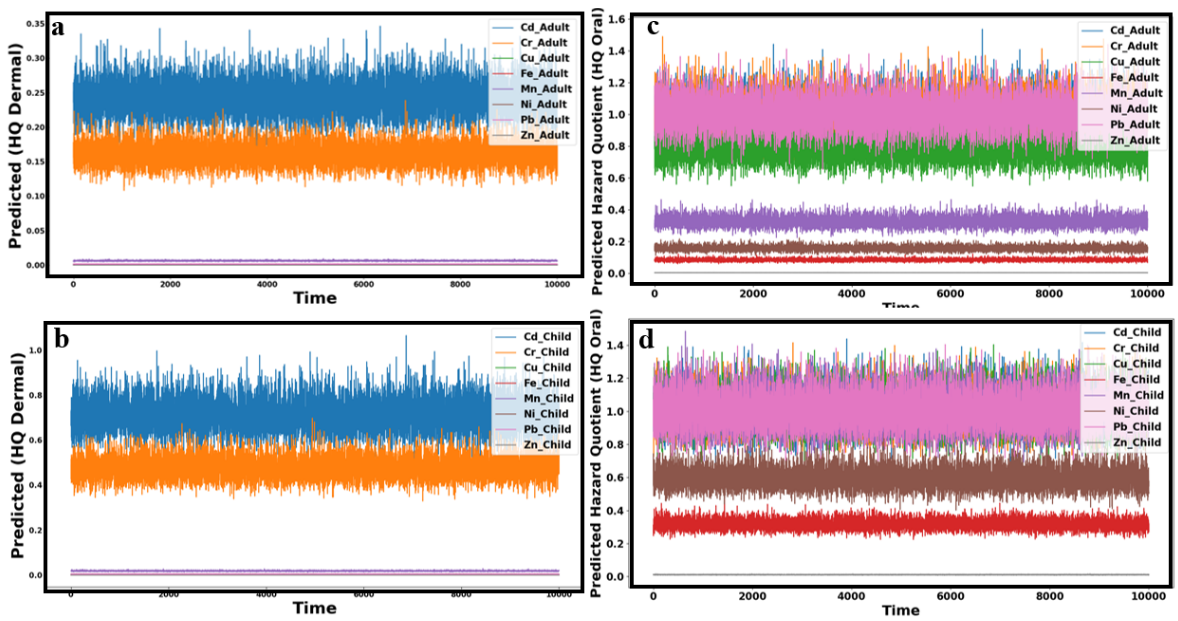

Figure 18. The predicted HQ dermal in old age group (adult) (a), $HQ_{predicted}$ dermal in young age group (child) (b), $HQ_{predicted}$ oral for adult (c), and $HQ_{predicted}$ oral for child.

Carcinogenic risk assessment (**Fig 19**) further confirmed the severity of the situation, with Cd, Cr, and Pb contributing to elevated cancer risk ($CR > 1\times10^{-4}$) in nearly all samples. Children again showed markedly higher susceptibility compared to adults, both for oral and dermal pathways. These findings emphasize the

long-term health implications of chronic exposure to contaminated water, particularly in regions where groundwater is the sole source for drinking and irrigation.
Monte Carlo simulations strengthened the reliability of these conclusions by accounting for variability and uncertainty in exposure parameters. The probabilistic models consistently identified Cd, Cr, and Pb as the dominant contributors to both non-carcinogenic and carcinogenic risks, confirming their role as priority contaminants requiring urgent mitigation. The simulations also demonstrated that predicted risk values closely matched calculated indices, validating the robustness of the approach for future risk assessment applications.

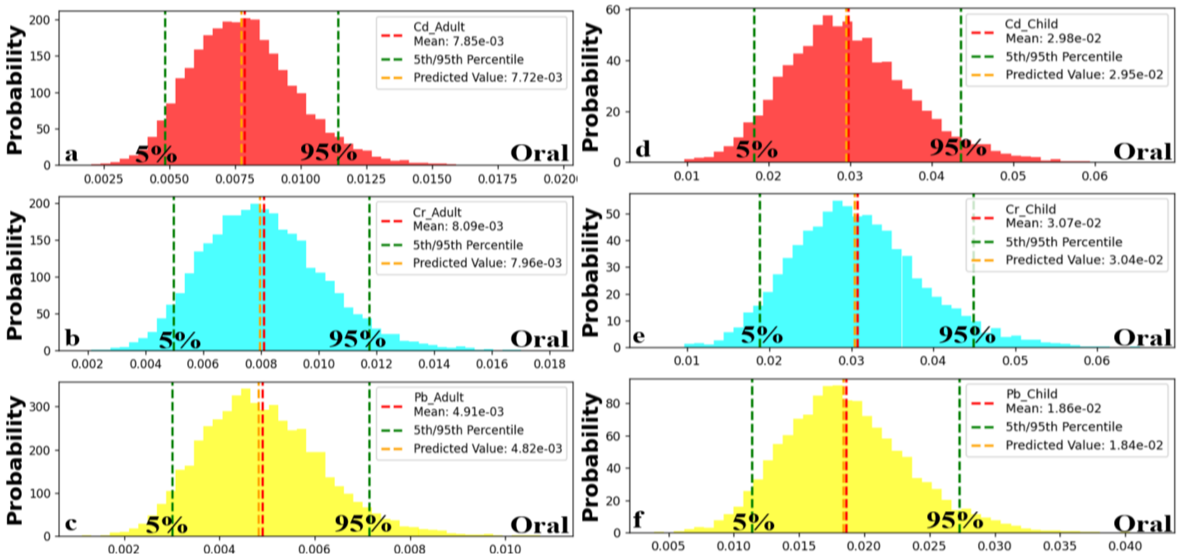

Figure 19. Predicted carcinogenic risk (CR) in adult (a, b and c) and child (d, e and f) through oral contact for Cd, Cr, and Pb respectively

5.7. Desalination of Brackish Water from the TCA Using Innovative Natural Material

This research presents a groundbreaking solution to the challenge of brackish water desalination by developing, synthesizing, and validating a novel, low-cost, and eco-friendly zeolite/geopolymer (Z/GP) membrane (**Fig 20**). By utilizing abundant, natural raw materials (kaolinite and diatomite), this study offers a practical and sustainable technological intervention to mitigate water scarcity and soil salinization in arid regions.
The primary new scientific result is the successful synthesis and exceptional performance of the Z/GP membrane, which achieved a salt rejection rate of over 99.8% and a water flux of up to 8.34 kg/m²/h. This demonstrates, for the first time, that a membrane derived from low-cost, natural geopolymers can achieve performance comparable to or exceeding that of more expensive, conventional polymer-based membranes. The key methodological advance was the hydrothermal conversion of a diatomite/kaolin geopolymer substrate into a multi-phase zeolite membrane (containing Zeolite-A, Zeolite-X, Sodalite, and Zeolite-P). This innovative synthesis process resulted in a highly porous, nanostructured material with a large surface area (106 m²/g) and optimal pore size (4.2 nm), which are the key factors behind its high desalination efficiency.
This work provides a powerful, practical solution to the problems identified in the preceding chapters. While previous sections quantified the extent of water quality degradation, this thesis provides a tangible technological solution. The study quantitatively clarifies the optimal operating parameters for the membrane, demonstrating that a thickness of 3 mm and a temperature of 75°C provide the best balance between high water flux (7.05 kg/m²/h) and near-perfect salt rejection (99.5%). Furthermore, the research provides quantitative evidence of the membrane's durability and reusability, showing stable performance over 130

hours of continuous operation and successful regeneration over multiple cycles, confirming its suitability for real-world applications.

The Z/GP membrane developed in this thesis is not just a solution for Siwa Oasis; it represents a paradigm shift in desalination technology for arid and developing regions worldwide. The use of locally sourced, inexpensive raw materials makes this technology highly accessible and economically viable for communities that cannot afford conventional, energy intensive desalination plants. The synthesis method is straightforward and scalable, offering a transferable blueprint for establishing local manufacturing of desalination membranes in other water-stressed countries. This research, therefore, provides a generalizable and sustainable pathway to water security, empowering communities to treat their own brackish water resources and break the cycle of water scarcity and soil salinization.

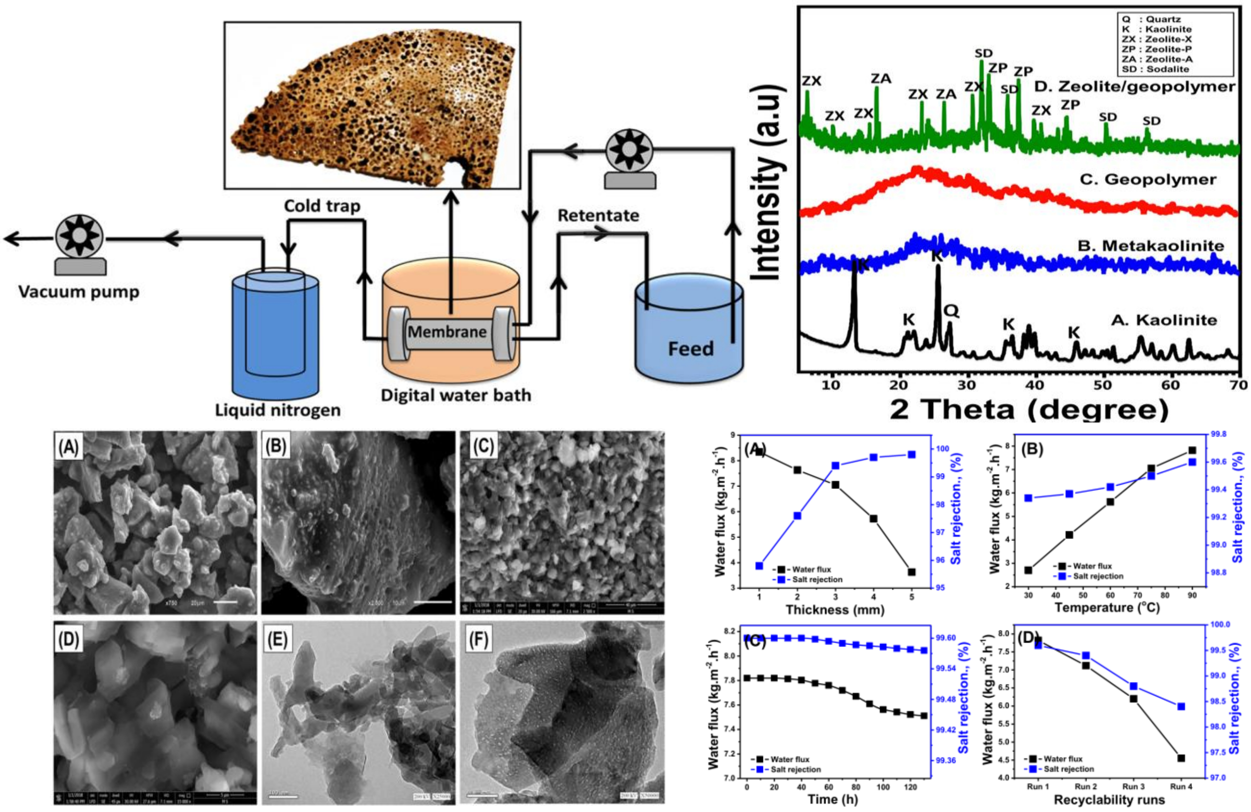

Figure 20. Schematic diagram of the pervaporation system used for desalination experiments with the synthetic Z/GP membrane. XRD patterns of raw kaolinite (A), metakolinite (B), synthetic D/K geopolymer (C), and the synthetic Z/GP membrane (D).

(A) SEM image showing the D/K geopolymer substrate, (B) SEM image illustrating the oriented pores within the D/K geopolymer, (C) SEM image of the Z/GP membrane highlighting its crystalline morphology, (D) SEM image depicting the porous matrix structure of the Z/GP membrane, (E) HRTEM image of the D/K geopolymer revealing its agglomerated particles and porous matrix, and (F) HRTEM image of the Z/GP membrane emphasizing its nanostructured porous material.

(A) Shows the influence of Z/GP membrane thickness on desalination performance, (B) the impact of feed temperature on the performance of the membrane, (C) the stability of the Z/GP membrane during a 130-hour desalination process, and (D) the recyclability of the prepared Z/GP membrane for reuse in desalination processes of Siwa brackish groundwater.

6. Conclusion

This PhD thesis provides a comprehensive diagnosis of the Siwa Oasis water crisis by integrating a suite of advanced methodologies, including machine learning, remote sensing, isotopic analysis, and numerical modeling. The research first constructed a high-resolution 3D geological model, identifying the critical fault systems that control the hydraulic connectivity between the deep, fresh Nubian Sandstone Aquifer (NSSA) and the shallow, brackish Tertiary Carbonate Aquifer (TCA). It then provided the first quantitative proof linking the expansion of agriculture over the past 30 years to the dramatic growth of hypersaline lakes, which, in turn, drive soil and groundwater salinization.

The study precisely quantified the mixing dynamics, revealing that the TCA's quality is governed by a delicate balance between upward recharge from the NSSA and downward leakage from saline lakes. Critically, the predictive numerical model forecasts a catastrophic reversal of the hydraulic gradient between the two aquifers within 150-200 years under current abstraction rates, which would irreversibly contaminate the region's only freshwater source. The research also highlighted significant health risks, particularly for children, from toxic elements in the water. As a practical solution, the study developed and validated a novel, low-cost geopolymer-zeolite membrane that demonstrated exceptional desalination performance. Ultimately, this work delivers an integrated, scientifically-grounded framework that not only explains the complex drivers of the water crisis in Siwa but also provides the predictive tools and technological solutions necessary for its sustainable management.

7. New Scientific results

This PhD thesis has undertaken a comprehensive, multi-disciplinary investigation of the Siwa Oasis hydrogeological system by integrating a wide array of advanced methodologies and diverse data sources. The research framework was designed to build a holistic understanding of the oasis's water resources, from their geological structure to their chemical composition and long-term sustainability. To achieve this, the study synergistically employed geophysical data (well logs, gravity, magnetics) with machine learning algorithms (SOM, K-means) to construct a high-resolution 3D geological model. Multi-temporal remote sensing data (Landsat) was analyzed using Support Vector Machines (SVM) to quantify land-use change and its environmental impacts. A suite of geochemical and isotopic tracers ($\delta^{2}H$, $\delta^{18}O$, ^{13}C, ^{14}C, $^{87}Sr/^{86}Sr$) were analyzed and interpreted using advanced statistical techniques (PCA, K-means) and inverse mixing models (NETPATH, Faure) to delineate recharge sources and quantify mixing processes. These empirical findings were then integrated into a predictive numerical flow model (FEFLOW) to simulate long-term aquifer behavior. Finally, the research developed and applied a novel IWQI, a probabilistic health risk assessment using Monte Carlo simulation, and synthesized an innovative zeolite/geopolymer membrane for desalination. The overarching aim of this integrated approach was to move beyond a descriptive analysis and to create a quantitative, predictive, and scientifically robust foundation for the sustainable management of groundwater in this critical arid ecosystem.
The application of this integrated methodology yielded seven key sets of findings concluded in 7 new scientific results as follows;

Thesis 1: Aquifer Characterization and Structure Controlling Aquifer System

the 3D geological model revealed the precise subsurface architecture and identified the fault systems that control the hydraulic connectivity between the deep NSSA and the shallow TCA. The SOM proved to be a highly effective and accurate method for delineating lithological units from well-log data, outperforming K-means in estimating the thickness of critical sand layers. The hydraulic properties of these units were validated, revealing hydraulic conductivity values ranging from 1.2 to 6.6 m/d, which are essential inputs for flow modeling. Furthermore, the analysis of gravity and magnetic data identified the dominant NE-SW, NW-SE, and E-W structural trends that control the groundwater flow system, confirming that deep faults in the NSSA act as conduits for upward recharge to TCA, while shallow fractures facilitate surface leakage. Finally, 3D gravity inversion provided a clear picture of the basin's architecture, mapping the basement depth from 2.5 to over 4.5 km.

Thesis 2: Soil Salinization Origin and mechanism controlling water chemistry

The study provided quantitative proof linking the 270% expansion of agriculture over 30 years to a 168% increase in the area of hypersaline lakes, identifying this as the primary driver of soil and water salinization. The main mechanism controlling water chemistry are calcite, dolomite, halite, gypsum dissolution, silicate weathering and ion exchange and evaporation. Geochemical modeling using PHREEQC identified mineral supersaturation conditions for montmorillonite, calcite, dolomite, and clay minerals that reduce soil permeability and increase waterlogging.

Thesis 3: Groundwater Recharge Source and Salinity Origin

The research confirmed a dual-source mixing model for the TCA, quantifying the respective contributions of upward leakage from the fresh NSSA and downward seepage from the saline lakes. Stable isotope analysis revealed that both the NSSA and TCA contain paleo-meteoric water. NETPATH mixing model quantified that hypersaline lakes contribute 0.6-4% to TCA salinity through downward seepage with the highest contribution from Zeitun lake, while NSSA provides 63-87% freshwater contribution through upward flow.

Thesis 4: Residence Time Estimation and Recharge Location of the TCA from NSSA

by combining multiple isotopic tracers, the study estimated the residence time of the groundwater and validated the fault-controlled recharge pathways. The Faure mixing model successfully quantified NSSA contributions to TCA recharge, demonstrating 80-90% NSSA input in low-salinity areas (1000-2000 mg/L) along fault planes, 50-80% in intermediate zones (2000-5000 mg/L), and minimal contributions (0-40%) in high-salinity northern regions (5000-9000 mg/L) near salt lakes. Groundwater age correction using radiocarbon dating revealed significant temporal variations with TCA ages ranging from 640-13,551 years and NSSA ages from 4,296-14,184 years, showing a clear spatial trend of decreasing age from southeast to north, with youngest ages near Siwa Lake indicating active mixing and recharge processes.

Thesis 5: Numerical flow model using backward particle tracking

The numerical flow model demonstrated critical drawdown patterns from 1960-2025, showing dramatic water level decline from 175m to 75m in western areas and slower decline from 142m to 128m in eastern regions, with future predictions indicating water levels will drop to 30-70m by 2100 under current extraction rates of 330,000 m^3/day. Reverse particle tracking analysis provided definitive validation of NSSA to TCA recharge mechanisms along distinct fault and fracture pathways confirming the findings of mixing models. The pathlines reaches the salt lakes confirming the leakage downward of salt lakes to the TCA.

Thesis 6: Water Quality and Health Risk Assessment of Potential Toxic Elements

The IWQI identified areas with extremely poor water quality, particularly in the TCA, due to high salinity. FFBP-NN effectively predicted water quality with high accuracy, reducing the need for extensive testing of many parameters. The health risk assessment highlighted significant non-carcinogenic and carcinogenic risks, especially for children, from exposure to cadmium, chromium, and lead.

Thesis 7: Desalination of Brackish Water from the TCA Using Innovative Natural Material

This study developed a geopolymer-based zeolite membrane from natural kaolinite and diatomite for desalination of the brackish water of the TCA after mixing with NSSA. The membrane showed impressive salt rejection (99.5%) with excellent thermal stability. This innovative desalination approach provides a sustainable solution for groundwater salinization in arid regions, offering an eco-friendly, cost-effective method for improving water quality in the Siwa Oasis and similar areas.

8. Practical applicability

The findings of this study provide critical insights for sustainable water management, particularly in arid regions like the Siwa Oasis, where understanding the complex interactions influencing water chemistry is essential for long-term resource conservation. Based on the results, the following scientifically-backed recommendations are proposed to optimize the quality, quantity, and sustainability of both water resources and soil fertility (**Fig 65**):

a) Dilution of groundwater salinity through mixing freshwater from the NSSA with brackish water from the TCA on the ground surface using a piped system

b) Desalination of the mixed water to the acceptable level of irrigation water to avoid further soil salinization.

c) Application of subsurface drip irrigation instead of flood irrigation to avoid further increase in the surface area of the salt lakes and protect the limited water resources.

d) Construct a drilling canal to connect the four major salt lakes and discharge their water into an artificial lake lined with impermeable material in the eastern part of Zeitun Lake. This would prevent hypersaline water from seeping into the TCA, reduce the salinity and surface area of hypersaline lakes, and create opportunities for economic and ecological benefits. The artificial lake could be divided into a fish pond and an evaporation pond, supporting aquatic life and salt production.

e) Implement a drainage system with cement-covered drains and perforated pipes to remove waterlogged soil and discharge it into the main lakes and drains.

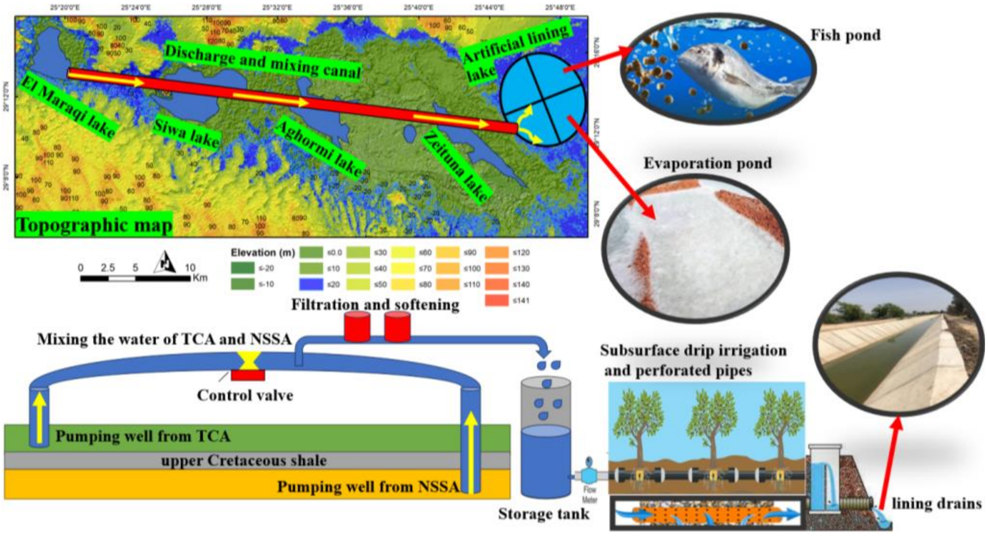

Figure 65. Schematic diagram of the recommended solutions in Siwa Oasis for sustainable development.

9. Author individual scientific works

Some of the journal papers

1. Eid, M.H.; Kovács, A.; Szűcs, P. Application of Stable Isotopes, Mixing Models, and K-Means Cluster Analysis to Detect Recharge and Salinity Origins in Siwa Oasis, Egypt. *Groundwater for Sustainable Development* **2024**, *25*, 101124, doi:10.1016/j.gsd.2024.101124.

2. Eid, M.H.; Kovacs, A.; Szűcs, P. Comprehensive Approach Integrating Remote Sensing, Machine Learning, and Physicochemical Parameters to Detect Hydrodynamic Conditions and Groundwater Quality Deterioration in Non-Rechargeable Aquifer Systems. *Heliyon* **2024**, *10*, e32992, doi:10.1016/j.heliyon.2024.e32992.

3. Eid, M.H.; Kovács, A.; Szűcs, P. An Advanced Approach for Drinking Water Quality Indexing and Health Risk Assessment Supported by Machine Learning Modelling in Siwa Oasis, Egypt. *Journal of Hydrology: Regional Studies* **2024**, *56*, 101967, doi:10.1016/j.ejrh.2024.101967.
4. Eid, M.H.; Tamás, M.; Kovács, A.; Szűcs, P. New Approach into Human Health Risk Assessment Associated with Heavy Metals in Surface Water and Groundwater Using Monte Carlo Method. *Sci Rep* **2024**, *14*, 1008, doi:10.1038/s41598-023-50000-y.

5. Eid, M.H.; Mikita, V.; Kovács, A.; Szűcs, P. Monte Carlo Simulation and PMF Model for Assessing Human Health Risks Associated with Heavy Metals in Groundwater: A Case Study of the Nubian Aquifer, Siwa Depression, Egypt. *Front. Earth Sci.* **2024**, *12*, 1431635, doi:10.3389/feart.2024.1431635.
6. Eid, M. H., Kovács, A., & Szűcs, P. (2025). Integrating Unsupervised Machine Learning, Statistical Analysis, and Monte Carlo Simulation to Assess Toxic Metal Contamination and Salinization in Non-Rechargeable Aquifers. *Results in Engineering*, 104989.
7. Eid, M. H., Kovács, A., Szűcs, P., Abukhadra, M. R. (2025). Calcium modified mesoporous silica from marble for the removal of cadmium, lead, chromium, iron, and manganese from Siwa Oasis groundwater. *Scientific Reports*, *15*(1), 31299.
8. Hemida, M. H. E., Szűcs, P., & Kovács, A. (2022). Problems threatening sustainability in Siwa Oasis and recommendations for understanding the sources of water quality deterioration. *GEOSCIENCES AND ENGINEERING: A PUBLICATION OF THE UNIVERSITY OF MISKOLC*, *10*(15), 138-153.
9. Eid, M. H., Mikita, V., Bence, C., & Szűcs, P. (2025). A novel integration of self-organizing maps and NETPATH inverse modeling to trace uranium and toxic metal contamination risks in West Mecsek, Hungary. *Journal of Hazardous Materials*, 139291.
10. Eid, M. H., Szűcs, P., Kovács, A., (2025). Impacts and sources of potential toxic elements on water quality and optimizing machine learning models for sustainable management. *Modeling Earth Systems and Environment*, *11*(5), 375.
11. Eid, M. H., Saeed, O., Szűcs, P., (2025). Seasonal hydrochemical characteristics of spring water in Southern Poland: integrating geochemical modeling, health risk analysis and mitigation strategies. *Scientific Reports*, *15*(1), 25459.
12. Eid, M. H., Awad, M., Mohamed, Szűcs, P. (2024). Comprehensive approach integrating water quality index and toxic element analysis for environmental and health risk assessment enhanced by simulation techniques. *Environmental Geochemistry and Health*, *46*(10), 409.
13. Eid, M. H., Tamma, A. A., Szűcs, P. (2024). Advanced approach combines integrated weight water quality index and potential toxic elements for environmental and health risk assessment supported by simulation technique in Oued Souf, Algeria. *Scientific Reports*, *14*(1), 17805.
14. Eid, M. H., Tamma, A. A., Péter, S. (2023). Evaluation of groundwater quality for irrigation in deep aquifers using multiple graphical and indexing approaches supported with machine learning models and GIS techniques, Souf Valley, Algeria. *Water*, *15*(1), 182.

Conferences

1. Hydrogeochemical evaluation of groundwater and its suitability for drinking and irrigation using water quality index, statistical and geochemical modelling, north eastern desert of algeria, Conference: Interdisciplinary topics in mining and geology: XXII Conference of PhD Students and Young Scientists, June 29-July 01, 2022: book of abstracts at: Politechnika Wrocławska.
2. Evaluation of groundwater quality for irrigation purposes using multiple graphical and indexing approaches supported with machine learning models and GIS techniques; representative case study, 2nd Canadian IWA-Young Water Professional Conference 2023 Leading from the Future Jun 1-3, 2023 - Vancouver, BC, University of British Columbia, Vancouver, Canada.
3. Integration of Geochemical Modeling, Hydrodynamic Condition, and Change Detection Supported with Machine Learning For Sustainable Development of the Water Resources in Western Desert, Egypt, AGU23 Conference 2023 Leading from the Future December 11-15, 2023 - San Francisco, CA, USA, Moscone center.
4. Monte Carlo Simulation and Multivariate Statistical Analysis for Environmental and Health Risk assessment of Heavy Metals in surface water and groundwater supported with python code: A Case Study of Siwa Oasis, Egypt, AGU23 Conference 2023 Leading from the Future December 11-15, 2023 - San Francisco, CA, USA, Moscone center
5. Comprehensive Approach to Detect the Salinity Origin and Recharge Source of Groundwater Using Stable Isotopes, Mixing Models, PCA, and K-Means Cluster Analysis, IWA-world water congress& exhibition. 2024. August 11-18, 2024 – Toronto, Canada.