CHAPTER 5

Modern information technologies in irrigation water quality assessment

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Abstract

Comprehensive evaluation of irrigation water quality is an important precondition for sustainable crop production on irrigated lands. Neglecting water quality monitoring can cause soil health deterioration, fertility loss, toxic effects on plants, reduced yield quality, and a decline in cropland productivity.

Comprehensive control of irrigation water quality, especially when the source is doubtful, requires time, specialized knowledge, and qualified labor. Raw laboratory results from water sample analysis are often difficult for non-specialists to interpret. Therefore, scientific expertise is required to calculate agronomic indicators and interpret them correctly. However, such expertise is not always available or affordable. As a result, the gap between scientific water quality assessment and practical implementation remains wide.

The main aim of this study is to introduce WaterQ AI, a web-based platform for rapid, scientifically grounded, and comprehensive analysis of irrigation water quality. The application was developed using a modern web development stack and scientific logic for the calculation and interpretation of 16 agronomically important irrigation water parameters using only pH and ion concentrations as input data. The platform covers indicators related to salinity, sodicity, alkalinity, water permeability, toxic ion effects, and the balance of major cations and anions (such as sodium adsorption ratio, magnesium ratio, Kelly's ratio, etc.). Its web-based format makes the tool accessible without installation, supports use on different devices, and facilitates application in research, education, consulting, and farm-level decision-making.

The comparison of WaterQ AI calculations with manual expert calculations showed an extremely small discrepancy of less than 0.15%, confirming the

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reliability of the implemented logic. The platform provides rapid, scalable, consistent, and reproducible evaluation of irrigation water quality indicators, reducing the time and cost required for assessment. It transforms laboratory data into agronomically meaningful conclusions and identifies risks of secondary salinization, alkalization, soil structure degradation, reduced infiltration, and crop toxicity. Nevertheless, the application should be regarded as a decision-support tool, not a replacement for professional expertise in agricultural melioration. Human expertise remains essential in edge cases, when final measures must consider soil texture, drainage, irrigation method, crop sensitivity, climate, and local agricultural standards.

Keywords

Agriculture, coding, digitalization, environmental threats, information technologies, irrigation, monitoring, plant care, rule-based artificial intelligence, water quality, web development.

5.1 Introduction

Agriculture is one of the biggest consumers of freshwater. Almost 70% of global freshwater consumption belongs to agricultural usage [1]. Climate change resulted in dramatic shifts in the availability of water resources for agricultural purposes. Increased air and land surface temperatures lead to greater evapotranspiration and combined with strong winds and uneven precipitation distribution cause extreme drought events and general aggravation of aridity in susceptible regions of the planet. In this regard, irrigation becomes the most important and powerful instrument providing sustainable crop production in the conditions of global warming. To some extent, irrigation transformed from option to mandatory agrotechnological component that is the only guarantee of reasonable yields and food security [2]. Although its beneficial effects on crop yields, especially in arid and semi-arid climate, is undebatable, there are some ecological threats related to artificial water supply. They include water erosion, flooding, freshwater scarcity, technological pollution, adverse effects on soil and plant. And the latter effects are especially concerning in the situation when irrigation water quality is far from being perfect.

The main concerns related to irrigation harmful effects on soil include secondary salinity and sodicity. These threats are especially concerning in semi-arid and arid climate, though adverse effects of poor irrigation water quality on soil systems is observed worldwide [3]. Continuous usage of the irrigation water with high content of total dissolved salts (TDS) inevitably leads to their gradual accumulation in the arable layer of the irrigated soil. Salt accumulation, in its turn, leads to the deterioration of soil physical, chemical, mechanical, biological properties (suppression of favorable microbium), and finally results in fertility loss. Besides, if irrigation water contains toxic salts (especially chlorides and carbonates) or harmful elements like heavy metals, its usage directly harms cultivated plants and leads to the yield quality and quantity losses. High sodium content poses not only the threat of secondary salinity, but also sodification hazards. Soils with high sodium content lose their optimal structure because of replacement of calcium ions with sodium in soil absorbent complex, become easily crusted and poorly aired. Sodified soils have corrupted water filtration, block normal nutrients uptake by plants because of extreme osmotic pressure disbalance. Combined with high sodium toxicity, all these factors cause heavy yield losses, and if not addressed properly, may lead to complete degradation of soil [4]. In some cases, provided saline irrigation water leaching and high groundwater table, there is a risk of groundwater mixing up with the irrigation water, leading even to more unpredictable future outcomes for agricultural ecosystem [5].

Therefore, irrigation water quality monitoring, especially if it is initially known that the source of the water is doubtful, is essential for sustainable irrigated agriculture. Although most farmers understand the hazards, they tend to neglect continuous monitoring of irrigation water quality because this procedure requires costs, time, and the most important – special expertise (as comprehensive water quality analysis requires calculation and interpretation of dozens of different qualitative indicators) that is not always affordable and accessible. Thus, there is a gap between actual demand for irrigation water quality monitoring, and agricultural producers' capacities to perform it on continuous basis.

In order to address this issue, a rule-based artificial intelligence (AI) system called WaterQ AI has been developed. Its main purpose is to provide accurate and rapid water quality analysis and help farmers, researchers, and water management professionals make informed decisions about water usage and amelioration. By analyzing key water parameters, received after the laboratory investigation of water samples, the system outputs a comprehensive roadmap of water quality, possible threats to soil and plant, as well as a clear guidance on how to avoid or minimize possible hazards. WaterQ AI is an example of deep integration between agro-industrial complex and modern information technologies, including AI-based automation systems, within the framework of so-called "digital precision agriculture" that is a rapidly developing branch and is projected to replace conventional agriculture in the nearest future.

5.2 Science behind WaterQ AI

WaterQ AI is a rule-driven system of irrigation water quality analysis. The application utilizes internationally accepted computation formula to evaluate the indicators of water quality and then applies hard-coded rules for their interpretation based on the corresponding scientific guidelines. Currently, WaterQ AI focuses mainly on the evaluation of agronomic criteria. The evaluation req uires inputs – therefore, user still will require to collect water samples and analyze them at any certified laboratory. Also, if user has no idea about general soil properties such as texture class, acidity level and buffer capacity, it is recommended to collect soil samples and analyze them too. Generally, the workflow of the application could be depicted in the following chart (**Fig. 5.1**).

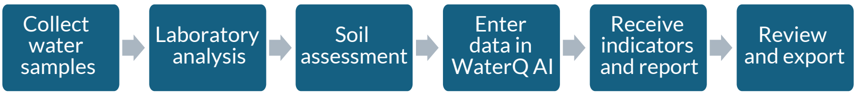

Fig. 5.1 WaterQ AI workflow chart

It is important that laboratory analysis of water samples include such parameters as concentrations of calcium (Ca^{2+}), magnesium (Mg^{2+}), sodium (Na^{+}), potassium (K^{+}), sulfate (HCO_3^{-}), chloride (Cl^{-}), carbonate (CO_3^{2-}), bicarbonate (HCO_3^{-}) ions in meq/L, and pH value. After laboratory analysis arrival, user must enter all the laboratory results and soil properties into the corresponding fields in the WaterQ AI dashboard. All ion concentrations must be in milligram-equivalents per liter (meq/L). In case that laboratory results are in different units, ensure that the values are converted in meq/L before entry. There are special links for relevant converters directly in the application guidelines section.

When the data are entered, WaterQ AI performs basic validation to ensure all inputs are valid numbers and within acceptable ranges. If validation successful, the application performs calculations using the guidelines to convert ions to salts, sort out toxic and non-toxic salts, evaluate different water quality indicators, namely:

1. Total Dissolved Salts (TDS) – the concentration of inorganic salts, dissolved in irrigation water samples, that determines general salinity hazard of irrigation water and indicates the potential risk of secondary soil salinization under continuous long-term irrigation. The calculation of the TDS content is based on the ions equilibrium and their interaction (that changes depending on the ions concentrations and relative shares). It must be noted that all the salts, excluding calcium sulfate and calcium

bicarbonate, are considered to be toxic to some extent, with the highest toxicity attributed to sodium carbonate and chloride salts.

2. Sodium Adsorption Ratio (SAR) – a widely used sodification indicator that evaluates relative dominance of sodium (Na^+) ions over calcium (Ca^{2+}) and magnesium (Mg^{2+}) ions, and point out at the risks of soil particle dispersion, aggregate breakdown, reduced infiltration, and general soil structure deterioration [6]. SAR is calculated using the equation (5.1)

$$SAR = \frac{Na^+}{(\sqrt{Ca^{2+} + Mg^{2+}})/2}. \quad (5.1)$$

3. Residual Sodium Carbonate (RSC) – the indicator of alkalinity and sodification hazards that focuses mainly on carbonate and bicarbonate ions dominance over calcium and magnesium ions [7]. RSC calculation is an additional metric to SAR and performed using the equation (5.2)

$$RSC = HCO_3^- + CO_3^{2-} - Ca^{2+} - Mg^{2+}. \quad (5.2)$$

4. Permeability Index (PI) – the indicator that is used to evaluate irrigation water effects on soil water permeability and infiltration capacities, points out on the risks of soil surface crusting, crops waterlogging, and puddle formation after irrigation [8]. The indicator is calculated using the equation (5.3)

$$PI = \left[\frac{Na^+ + \sqrt{HCO_3^-}}{Ca^{2+} + Mg^{2+} + Na^+}\right] \times 100. \quad (5.3)$$

5. Toxic Ions Concentration (eCl) – the indicator that reflects the risks of direct toxic effects of irrigation water on plants, especially from chloride and carbonate ions [9]. The chloride equivalent of toxic ions in irrigation water is calculated using the equation (5.4)

$$eCl = Cl^- + 0.2SO_4^{2-} + 0.4HCO_3^- + 5CO_3^{2-}. \quad (5.4)$$

6. Soluble Sodium Percentage (SSP) – the indicator that additionally establishes the dominance of sodium over other ions and reflects the effects of water on soil sodification hazards [9]. It is calculated using the equation (5.5)

$$SSP = \frac{Na^+}{Na^+ + K^+ + Ca^{2+} + Mg^{2+}} \times 100\%. \quad (5.5)$$

7. Stebler's Alkaline Coefficient (K) – reflects the risks of secondary soil salinization and alkalization caused by unfavorable proportions of ions [10]. Depending on the ratio of ions in the water sample, it is calculated using the system of equations (5.6)–(5.8):

$$K = 2040/Cl^{-};\tag{5.6}$$

$$K = 6620/(Na^{+} + 2.60Cl^{-});\tag{5.7}$$

$$K = 662/(Na^{+} - 0.32Cl^{-} - 0.43SO_4^{2-}).\tag{5.8}$$

8. Coefficient of Ion Exchange (CIE) points out at the balance between flocculating and dispersing ions that is important for understanding irrigation water effects on soil physical and chemical properties [11]. CIE is calculated using the equation (5.9)

$$CIE = (Ca^{2+} + Mg^{2+})/Na^{+}.\tag{5.9}$$

9. Kelly's Ratio (KR) – the indicator of sodium dominance over calcium and magnesium ions, determines the risks of damage to soil structure, physical and chemical properties [12]. The calculation is performed using the equation (5.10)

$$KR = Na^{+}/(Ca^{2+} + Mg^{2+}).\tag{5.10}$$

10. Thermodynamical Coefficients – the indicators that describe the physicochemical behavior of irrigation water and dissolved ions, useful for evaluating the risks of carbonate precipitation, changes in ion dominance, alkalinity development risks, as well as the long-term interaction peculiarities between irrigation water and soil [9]. Calcium potential (or sodification indicator) is calculated using the equation (5.11). Alkalinity potential is calculated using the equation (5.12), while the indicator of buffer capacity is calculated using the equation (5.13):

$$pNa - 0.5pCa;\tag{5.11}$$

$$pH - pNa;\tag{5.12}$$

$$\frac{pH - pNa}{pNa - 0.5pCa}.\tag{5.13}$$

11. Aydarov-Golovanov Coefficient (AGC) – the integrative indicator of the "soil – water – salt regime" in the field that is used to characterize the risks of adverse changes in salinity and alkalinity of the irrigated soil [13]. This indicator is calculated by the equation (5.14)

$$AGC = Na^{+} \times \frac{100\%}{Ca^{2+} + Mg^{2+}}. \quad (5.14)$$

12. Magnesium Ratio (MR) points out at the dominance of magnesium over calcium ions, determines likelihood of negative magnesium effects on soil structure, alkalinity, and some structural properties [9]. The indicator is calculated using the equation (5.15)

$$MR = Mg^{2+} / Ca^{2+}. \quad (5.15)$$

In addition to the listed indicators, irrigation water samples are analyzed by raw pH values, raw concentrations of ions, and final verdict about irrigation water acceptability and usage recommendations are given considering the entered soil properties.

The final report includes 16 different agronomic indicators of irrigation water quality, each with its own classification and description:

– excellent: irrigation water is safe for all irrigation purposes;

– good: irrigation water is suitable in most scenarios;

– fair: irrigation water has limited suitability, and careful dynamic monitoring for soil meliorative status is required;

– poor: irrigation water usage is restricted because it is unsafe to apply it without proper amelioration measures;

– unsuitable: irrigation water should be avoided in crop production.

The complete list of water quality indicators includes total dissolved solids (TDS), pH, toxic ions content (eCl), carbonates and bicarbonates content, soluble sodium percentage (SSP), sodium adsorption ratio (SAR), residual sodium carbonate (RSC), Kelly's ratio (KR), alkalization hazard, Stebler's ratio (K), cation exchange index (CIE), magnesium ratio (MR), permeability index (PI), corrosion ratio (CR), Aydarov-Golovanov coefficient (AGC), thermodynamic indicators (solubility product and ion activity).

Of course, WaterQ AI interpretations and recommendations should be revised by a specialist taking into account full specter of soil properties, crop structure, agrotechnology, land reclamation measures taken, etc.

5.3 Technical stack and development

Initially, WaterQ AI was launched as a command-line interface (CLI) interactive chatbot written in Python 3, with minimal requirements for external libraries. This approach allowed the rapid implementation and testing of the core scientific logic of the application, including the calculation of irrigation water quality indicators and rule-based interpretation of agronomic risks.

Later, a simple graphical user interface (GUI) with multilingual support was introduced to improve the user experience (UX), since CLI applications often appear unfamiliar, inconvenient, or technically complicated for non-specialist users. Inno Setup was used to create an installation package that included all required libraries and the Python runtime itself. This was important because many potential users do not have Python 3 pre-installed and may not know how to configure the runtime environment or install additional dependencies manually [14].

However, this desktop-based implementation still had several limitations. The application depended on the user's operating system (OS), Python version, and library compatibility. In addition, the installer file was relatively large, even though the application script itself was small. These limitations reduced the portability and accessibility of the software, especially for users with limited technical skills or restricted access to administrative rights on their computers.

Therefore, it was decided to rebuild the application as a web-based software tool, while preserving the same core scientific rule logic developed in the initial Python version. This transition solved several practical problems at once.

First, web development made it possible to provide a more visually attractive, intuitive, and user-friendly interface with less effort compared with maintaining separate desktop versions for different operating systems.

Second, the web application can be accessed from any internet-connected device, including desktop computers, laptops, tablets, and smartphones.

Third, distribution and user access are much easier for a web application, since users do not need to install software, configure dependencies, or update local packages manually.

The web version of WaterQ AI was developed using TypeScript and the React 18 framework. TypeScript was selected because it improves code reliability through static typing, which is especially important for scientific and calculation-based applications where incorrect data types or formula implementation errors may lead to misleading results. React 18 was used to build a modular, component-based interface that supports future expansion of the application, including the addition of new water quality indicators, multilingual content, explanatory blocks, and visualization components. The react-i18next library was implemented to provide smooth support of multiple languages.

The web-based architecture also improved the scalability and maintainability of the project. Separate interface components can be developed for data input, calculation results, water quality classification, agronomic interpretation, and user guidance. This makes the application easier to update and extend compared with the earlier monolithic desktop script. Moreover, the same scientific calculation logic can be reused across different interface elements, ensuring consistency between numerical outputs, textual explanations, and final recommendations.

Special attention was paid to UI/UX design. The web interface was made responsive and adaptable to different screen sizes, allowing users to work with the tool on both large monitors and mobile devices. This is particularly important for agricultural consultants, researchers, students, and practitioners who may need to access the application directly in field conditions or during consultations. Compared with the CLI and desktop versions, the web application provides a clearer workflow: users enter hydro chemical parameters, the system calculates irrigation water quality indicators, and the results are presented in an understandable format with agronomic interpretation.

Another important advantage of the web version is its accessibility for demonstration, education, and dissemination. Since the application is available through a direct link, it can be easily shared with farmers, students, researchers, advisory services, and potential stakeholders. This significantly increases the practical value of the tool and supports its use not only as a calculation engine, but also as an educational and decision-support platform for irrigation water quality assessment. Besides, built-in forms for feedback and getting in touch with the developer provide great opportunity for users to participate in further development process through bug reporting or retrieving explanations about the application functionality.

Thus, the transition from a Python-based CLI/desktop application to a TypeScript and React-based web application allowed WaterQ AI to preserve its scientific calculation core while becoming more accessible, scalable, user-friendly, and suitable for wider practical implementation. The application is available at: https://waterqai.web.app/.

5.4 WaterQ AI vs manual expertise

As far as WaterQ AI is a universal tool that is used by scientists and farmers, it is important to ensure that the results of water quality evaluation are reliable.

To perform a scientific evaluation of the application's performance, actual data on water quality analysis in the river Dnipro and the Ingulets irrigation system main channel were subjected to WaterQ AI and manual expertise. The results of both water quality evaluations are presented in **Table 5.1**.

Table 5.1 Comparison of WaterQ AI and manual expertise in irrigation water quality analysis

No.	Manual expertise results				
	TDS, mg L^{-1}	KR	SAR	SSP, %	PI, %
1	560	0.31	1.09	23.65	45.80
2	2008	0.95	5.50	48.80	54.20
3	1471	0.88	4.30	47.20	55.00
	WaterQ AI analysis results ± residuals				
1	559.48 ± 0.52	0.31 ± 0	1.09 ± 0	23.65 ± 0	45.40 ± 0.40
2	2004.90 ± 3.10	0.95 ± 0	5.50 ± 0	48.84 ± 0.04	54.18 ± 0.02
3	1470.30 ± 0.70	0.88 ± 0	4.33 ± 0.03	46.67 ± 0.53	54.97 ± 0.03

It was established that there was almost no discrepancy between such indicators of irrigation water quality as Kelly's Ratio and SAR; subtle differences were found for Sodium Percentage and Permeability Index, while the biggest differences were recorded in TDS content assessment (reached 0.15% as the highest). Considering the neglectable difference in calculation results, it could be pointed out that WaterQ AI provides robust and reliable scientifically grounded computation of agronomic criteria, extending raw indicators to interpretable numbers.

In addition, core advantages and major limitations of WaterQ AI, compared to manual expertise, were listed in **Table 5.2**. Key evaluation metrics, considered to be of the most importance for scientific web application, included accuracy and precision, misinterpretation hazards, speed, cost-effectiveness, consistency and reproducibility, coverage of multiple indicators, transparency of evaluation, adaptability of interpretations, scalability. Each dimension was assessed using a three-point scale (the higher – the better), and a total cumulative effectiveness score was calculated.

As a result of comparison, WaterQ AI is a winner. However, in the fields of adaptability to certain agro-industrial conditions, misinterpretation hazards and transparency of water quality assessment, the system will be beaten by manual expertise, conducted by professionals in land reclamation and agricultural melioration.

Therefore, WaterQ AI is more of a helpful tool rather than human replacement. Alongside modern machine learning (ML) based instruments for irrigation water quality prediction, it greatly improves organizational and economic component of meliorative analysis [15]. While different ML-driven tools are mainly directed to project further changes in irrigation water quality indicators based on the historical series of data with the highest possible precision (some models have the values of the coefficient of determination exceeding 0.98) [16], WaterQ AI focuses on automation of water quality assessment using the battery of various indicators. This feature makes the developed application a unique example of agricultural melioration automation.

Table 5.2 Advantages and limitations of WaterQ AI in irrigation water quality analysis

Metrics	WaterQ AI	Manual expertise
Accuracy and precision	+++	+++
Misinterpretation hazards	++	+++
Speed	+++	+
Cost-effectiveness	+++	+
Consistency and reproducibility	+++	++
Coverage of multiple indicators	+++	++
Transparency of evaluation	++	+++
Adaptability of interpretations	+	+++
Scalability	+++	+
Total score	23	19

Further improvements of WaterQ AI will be directed on the extension of the application functionality with additional irrigation water quality analysis domains, specifically, toxico-ecological and sanitary-hygienic indicators. For example, heavy metals pollution index (HPI), Nemerow pollution index (NPI), potential ecological risk index (PERI), heavy metal evaluation index (HEI), pollution load index (PLI), and modified degree of contamination index (mCd) will be embedded in the application workflow [17]. In addition, such parameters as biochemical oxygen demand (BDO) [18], pesticides and oil products content will be included in the algorithm for comprehensive irrigation water quality analysis. As for sanitary-hygienic domain, Escherichia coli total coliforms, intestinal helminths (nematodes), and specific pathogens such as Salmonella spp. and Listeria monocytogenes amounts as key sanitary indicators will be evaluated [19]. The evaluations will be accompanied by detailed recommendations on water quality improvement and restrictions on use. Introduction of all the mentioned indicators and features will be implemented within individual WaterQ AI sections, and will transform the application into a powerful all-around tool for robust automated assessment of irrigation water quality for different purposes.

5.5 Conclusions

WaterQ AI is a scientifically driven rule-based web platform that provides agricultural scientists and farmers with a comprehensive toolkit to perform rapid and precise evaluation of irrigation water quality by sixteen major indicators. The accuracy of calculations is not inferior to manual expertise, while the application saves much time and decreases costs for laboratory analysis interpretation, providing fast, scalable and consistent evaluation. However, the application has its limitations, mainly in terms of recommendations adaptability to different soil, climate, and agro-industrial conditions, as well as poses somewhat higher hazards of misinterpretation in edge cases. Therefore, WaterQ AI is not a replacement for agricultural experts – it is an assistant that helps to perform water quality analysis faster and cheaper without losing accuracy.

Conflict of interest

The authors declare that there is no conflict of interest in relation to this paper, as well as the published research results, including the financial aspects of conducting the research, obtaining and using its results, as well as any non-financial personal relationships.

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Data availability

Data will be made available on reasonable request.

Use of artificial intelligence statement

The authors confirm that they did not use artificial intelligence technologies when creating the current work.

Authors' contributions

Pavlo Lykhovyd: Conceptualization, Supervision, Writing – review & editing, Data curation, Investigation, Methodology, Writing – original draft, Software.

Gennadiy Karashchuk: Writing – original draft, Data curation, Project administration, Resources.

Elgudzha Kulidzhanov: Writing – original draft, Resources, Supervision, Formal analysis.

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