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A COMPUTATIONAL FRAMEWORK FOR PRECISION SPRAY-TANK ACIDIFICATION: AN INTEGRATION OF CHEMICAL EQUILIBRIUM MODELING AND INFORMATION TECHNOLOGIES TO ENSURE CHEMICAL STABILITY OF PESTICIDES

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Problem statement. Changes in agroecological conditions related to global warming have significantly shifted the reality of crop protection. Rapidly changing environmental conditions resulted in the aggravation of crop diseases, insects and weeds infestation. For example, increased air temperature and prolonged warm periods result in more rapid and intense propagation of various insects, because they have better winter dormance conditions (results in higher rates of overwinter survival), as well as faster passing main development stages and having more generations per season. Besides, higher temperatures result in intense migration of insects to new agroclimatic zones, widening the specter of host crops, making plant protection measures less effective and phytosanitary situation less predictable [14]. The combination of ecological factors and related changes in the biology of plant pathogens and weeds results in significant decrement of conventional plant protection measures.

Literature analysis. Mutation of the harmful insects also takes place at faster than usual pace, making traditional pesticides less effective to control them. In addition, some chemicals, e.g., popular pyrethroid insecticides, lose their efficiency in the conditions of hot weather (when air temperature rises above +25°C) that makes efficient control of insects even more complicated [11].

As for diseases, the situation is quite similar. Elevated levels of carbon dioxide in the atmosphere exacerbate the interactions between the host plants and pathogens (fungal, viral, etc.) that in its turn result in more complicated interactions in the “plant – pathogen” chain. Additionally, climate change resulted in dramatic shifts in pathogens spreading, and nowadays agrarians are facing the pandemic of recently unknown in their vicinity plant pathogens, which are aggressive, and difficult to control. New strains of pathogens are more resistant to available chemicals, as well as more virulent and dangerous for crops. Also, changes in air humidity and precipitation distribution, which accompany increased air temperature, alter usual pathways of pathogens spreading, infestation rates and patterns of disease manifestation [8]. Besides, some fungicides also may become less effective in new agroclimatic conditions that will make disease control tricky and challenging. According to recent scientific studies, this is mainly true for contact fungicides, especially in the agroclimatic zones where prediction of heavy showers and intense drought is complicated [16]. However, now there is no as convincing scientific evidence for fungicides efficiency decrease as for pyrethroids [7].

Weeds are another nightmare of plant protection specialists. They can cause yield losses up to 34%, which is almost twice as high as average losses from insects (18%) and diseases (16%) [13]. In the conditions of climate change, there is strong scientific evidence for the increased weed-related threats, as they tend to grow and spread faster. This makes weed control more challenging, especially taking into account that unfavorable weather conditions will make many popular herbicides less effective due to the modified activity and stability of chemical substances [5]. For example, recent research demonstrated the decreased efficiency of glyphosate herbicides [17]. And the reason is not only in the air temperature increase and moisture deficit (it is critical for some ground herbicides and those herbicides that require moist leaves surface for better penetration into the weed tissues) but is also related to the CO_2 concentration in the atmosphere because carbon dioxide has tremendous effects on weeds tolerance to chemical treatment [15]. That is why weed control is extremely complicated and require agrotechnological measures to enhance the efficiency of herbicides application in the challenging weather conditions.

Taking into account the mentioned above facts, it is evident that today effective plant protection has become more complicated and challenging as ever before. Besides, the concerns around massive pesticide application for crop protection are increasingly growing, and most people tend to be reluctant to consume plant products if they know that they were cultivated under heavy pesticide usage, as general awareness about harmful effects of chemicals on health and environment becomes deeper. In this regard, the simplest solution – increase frequence and dosage of pesticides to ensure appropriate level of pest control – is not considered as a way of improving the situation in plant protection. Modern crop protection faces two major challenges: effective control of phytopathogens and weeds in the context of global warming, and simultaneous need to minimize pesticide usage as much as possible [6].

In addition to general challenges, which were described earlier, Ukrainian farmers face another complication that is related to water quality used for spray-tank mixture preparation. It is a well-established fact that most traditional chemical pesticides require neutral or slightly acid pH of the tank mixture to provide the best efficiency. In alkaline water, they tend to degrade through hydrolysis, and as a result, lose their effectiveness [2]. Most farmers, especially those in the South of Ukraine, who are working on the Igulets irrigation land array, have no option but use the alkaline water (with pH values about 8.0 and even higher in some periods of the growing season) to prepare spray-tank mixture [9]. Therefore, this is an additional source of pesticide efficiency decrease. To mitigate adverse effects of alkaline water on pesticides, one can use safe amendment – physiologically acid fertilizers. They are safe for plants and environment, and in proper doses will reduce the pH of spray-tank to the required levels. The only drawback of this method is that agricultural practitioners have no idea about what amount of the fertilizer of certain type they must add to the spray-tank mixture to improve its chemical reaction.

Therefore, the main **purpose** of this study is to provide a scientific methodology for the usage of traditional physiologically acid fertilizers to acidify spray-tank mixture to the required pH levels based on the initial water pH and other influential factors, and develop a practical tool in the form of web and mobile application entitled AquaTune for farmers to make complicated chemical balance calculations automated and accessible for everyone.

Materials and methods. The development of the AquaTune application framework was divided into three primary phases: the establishment of a theoretical chemical equilibrium model, the curation of a stoichiometric fertilizer database, and the implementation of a cross-platform computational engine using modern programming technological stack for web and mobile development.

The core of the system relies on the quantitative assessment of water buffering capacity and the prediction of pH shifts following the introduction of acidifying fertilizers.

To account for the buffering capacity of alkaline carrier water, the model implements the Henderson-Hasselbalch equation adapted for the carbonate-bicarbonate system [10]. The primary equilibrium considered is the dissociation of carbonic acid H_2CO_3 using the following equation (1):

$$pH = pK_{a1} + log_{10}\left(\frac{HCO_3^-}{CO_{2aq}}\right) \quad (1),$$

where pK_{a1} is adjusted according to the temperature-dependent reaction kinetics described by the Van't Hoff equation [3], ensuring accuracy across diverse field conditions.

For long-term acidification (24-hour and extended-release modes), the engine incorporates a biological oxidation model. The model calculates the release of protons (H^+) esulting from the two-step nitrification process of ammonium-based fertilizers (NH_4^+):

$$NH_4^+ + 2O_2 \rightarrow NO_3^- + H_2O + 2H^+ \quad (2)$$

The framework estimates the potential pH drop based on the stoichiometric release of two moles of acidity per mole of oxidized nitrogen, adjusted for the theoretical rate of microbial activity in the spray tank or soil-water interface.

A comprehensive library of physiologically acidic fertilizers was compiled. For each entry, the following "Materials" parameters were recorded:

1) Acidity Coefficients: Defined as the centimoles of H^+ produced per gram of fertilizer;

2) Solubility Products (K_{sp}): The index used to evaluate the risk of sedimentation, especially for calcium phosphate and calcium sulfate;

3) Purity and Nutrient Density: Stadard molecular weights and nutriehts content in percents;

4) Tentative Price: Used to determine the economic effectiveness of the fertilizer fpr spray-tank mixture acidification.

The AquaTune software was developed to solve a multi-objective optimization problem: identifying the fertilizer combination that achieves the target pH at the lowest economic cost while remaining below the safety threshold for phytotoxicity and precipitation.

The technological stack of AquaTune engine was implemented in TypeScript (for the React 18 web interface) and Kotlin (for the Android Jetpack Compose application). To ensure scientific consistency, both platforms utilize an identical algorithmic core, preventing "platform drift" in recommendations. The system utilizes a conditional logic gate to flag incompatible mixtures (e.g., mixing calcium-based fertilizers with sulfates or phosphates) based on documented chemical compatibility charts.

To validate the computational outputs, a standardized "Jar Test" protocol was integrated into the workflow. This allows for empirical verification of the model's predictions:

Baseline Measurement: Determination of initial water pH and alkalinity.

Simulated Application: Addition of the AquaTune-calculated dosage to a 1L sample.

Kinetic Observation: pH measurement at T=0 (immediate) and T=24h (biological) to correlate field results with theoretical models.

Results. The AquaTune framework demonstrates a significant advancement in digital precision agriculture by operationalizing complex chemical models into a real-time decision-support tool for plant protection efficiency enhancement. Unlike traditional "rule-of-thumb" methods – such as the manual "eyedropper jar test" commonly recommended by extension services – AquaTune utilizes a non-linear Henderson-Hasselbalch engine to predict pH shifts with high precision.

A key functional advantage is the dual-mode acidification approach. While most commercial acidifiers focus on immediate pH reduction, AquaTune accounts for biological acidification via nitrification. This is critical for fertilizers like Ammonium Nitrate (NH_4NO_3), where the secondary release of protons (H^+) during the oxidation of NH_4^+ can lead to unintended over-acidification if not accounted for by the initial dosage [1].

The results of the software implementation show a highly accessible interface that accommodates varying levels of technical expertise (Fig. 1):

Progressive Disclosure: The "Simple" vs. "Expert" modes ensure that entry-level farmers can achieve safe results, while researchers can adjust advanced parameters like temperature-dependent reaction kinetics.

Cross-Platform Performance: The synchronized engine between React/TypeScript and Kotlin ensures zero discrepancy in scientific outputs across devices, a common failure point in multi-platform agricultural software.

Global Localisation: By supporting four languages (English, German, Spanish, Ukrainian) and localized fertilizer pricing, the tool bridges the gap between theoretical chemistry and regional economic realities.

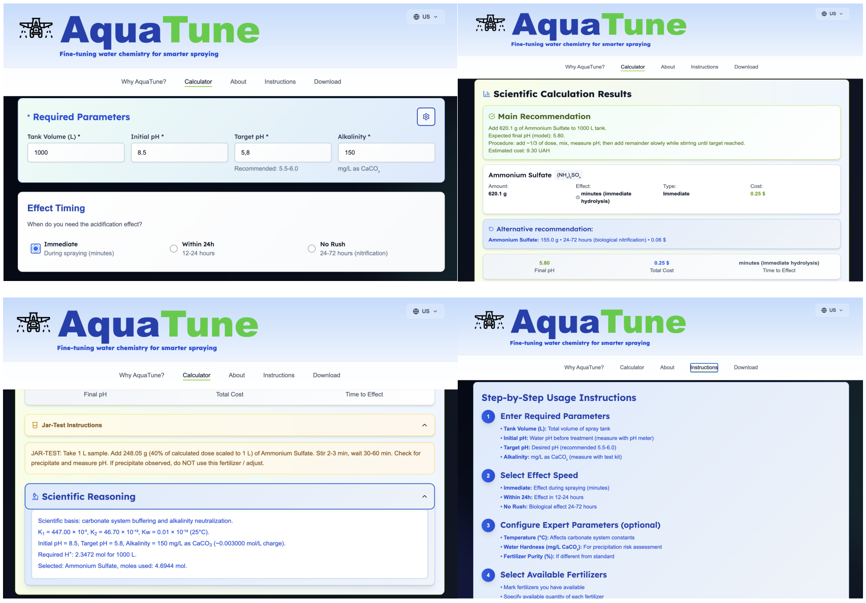

Fig. 1. AquaTune web application user interface

Current study and its results highlight a critical "knowledge-action gap" in spray-tank mixture's pH management. While scientific literature extensively documents the risks of alkaline hydrolysis – where pesticide half-lives can drop from days to minutes in water with pH > 8 and diminish their effectiveness in plant pathogens, insects and weeds control [4] – the available digital tools have remained remarkably simplistic.

A review of the current market and literature reveals that AquaTune is a unique application with no direct scientific analogues available.

For example, Tank Mix Calculator application available for smartphones provides farmers with a simple instrument for building compatible pesticide mistures for spraying but has nothing to do with adjustment of spray-tank water pH to optimize the efficiency of pesticides application.

Similarly, academic models of the carbonate system are typically confined to complex laboratory software rather than field-ready decision support mobile platforms. Notwithstanding the fact that various research showed the importance of spray-tank mixture pH optimization to ensure the best chemical protection effectiveness [12], there were no ready-to-use solutions until now. AquaTune effectively synthesizes agricultural and chemical science with farming practices and information technologies, providing the first integrated tool that combines chemical equilibrium, biological kinetics, and economic optimization for precision spraying.

Conclusions. The development of the AquaTune application represents reaching a significant milestone in the digital transformation of precision agriculture. By successfully integrating complex carbonate equilibrium chemistry and nitrification kinetics into a user-friedly mobile and web interface, this study demonstrates that sophisticated chemical modeling can be made accessible for daily on-farm decision-making. The use of the Henderson-Hasselbalch equation and temperature-corrected constants provides a statistically superior method for calculating target pH compared to conventional volumetric estimations. This prevents the chemical degradation of pesticides and maximizes their effectiveness. The automated precipitation risk assessment, based on solubility products and chemical compatibility logic, significantly reduces the likelihood of nozzle clogging and phytotoxicity. This ensures that the optimization of water chemistry does not come at the expense of equipment longevity or crop safety. By optimizing fertilizer combinations based on real-time pricing and stoichiometric efficiency, AquaTune enables farmers to achieve the desired water pH in a spray-tank at the lowest possible cost. Furthermore, by reducing chemical waste through improved application efficiency, the tool contributes to a more sustainable and environmentally responsible agricultural footprint. The synchronized cross-platform architecture (React/Kotlin) proves that high-fidelity scientific engines can operate reliably in offline environments, ensuring that advanced decision support is available even in remote agricultural regions. To sum up, AquaTune fills a critical void in the current agricultural software market. It moves beyond simple dosage calculators to provide a comprehensive, science-based solution for spray-tank management.

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Вожегова Р.А., Лиховид П.В., Лавренко С.О., Максимов Д.О. Обчислювальний фреймворк для точного підкислення бакової суміші: інтеграція моделі хімічної рівноваги та інформаційних технологій для забезпечення хімічної стабільності пестицидів

Мета. Запропонувати наукову методику використання традиційних фізіологічно кислих добрив для підкислення бакової суміші обприскувача до потрібного рівня pH виходячи з початкового pH води та інших факторів впливу, а також розробити практичний інструмент у форматі веб та мобільного додатку під назвою AquaTune для фермерів, щоб зробити складні розрахунки хімічного балансу автоматизованими та доступними для кожного.

Методи. В основі системи лежить алгоритмізація рівняння Гендерсона-Гассельбаха та температурно-залежної кінетики реакцій для формування стратегій високоточного підкислення. Виходячи за межі стандартних статичних калькуляторів, AquaTune унікально інтегрує кінетику нітрифікації, враховуючи біологічне вивільнення протонів (H^+) з часом для забезпечення довгострокової стабільності рівня pH. Платформа оперує базою даних розповсюджених фізіологічно кислих добрив, використовуючи стехіометричні константи та аналіз добутку розчинності для мінімізації ризиків випадання в осад поживних речовин та поломки обладнання. Для розробки використано сучасний веб та мобільний стек технологій програмування.

Результати. Завдяки синхронізованим обчислювальним механізмам із можливістю автономної роботи та багатомовному інтерфейсу, AquaTune забезпечує глобально доступне рішення для економічної та хімічної оптимізації бакових сумішей. Наші результати демонструють, що такий комплексний підхід не лише запобігає дороговартісній деградації хімічних компонентів, а й підвищує екологічну стійкість програм захисту рослин. AquaTune постає як унікальний, науково обґрунтований аналог традиційних об’ємних методів, що перетворює складне моделювання хімічної рівноваги на ефективний, готовий до використання в полі інструмент підтримки прийняття рішень.

Висновки. Розроблений додаток AquaTune інтегрує складні хімічні моделі карбонатної рівноваги та кінетики нітрифікації у зручний інтерфейс для точного землеробства. Це дозволяє фермерам оптимізувати склад робочих розчинів, запобігаючи деградації пестицидів і засміченню обладнання, що підвищує ефективність та екологічну стійкість господарства.

Ключові слова: кислотність, лужність, цифрове сільське господарство, застосування пестицидів, захист рослин, якість води.

Vozhehova R.A., Lykhovyd P.V., Lavrenko S.O., Maksymov D.O. A computational framework for precision spray-tank acidification: An integration of chemical equilibrium modeling and information technologies to ensure chemical stability of pesticides

Purpose. To propose a scientific methodology for utilizing traditional physiologically acidic fertilizers to acidify sprayer tank mixtures to the required pH level – based on initial water pH and other influencing factors – and to develop a practical web and mobile tool named AquaTune to automate complex chemical balance calculations for farmers.

Methods. The system is centered on the algorithmization of the Henderson-Hasselbalch equation and temperature-dependent reaction kinetics to formulate high-precision acidification strategies. Moving beyond standard static calculators, AquaTune uniquely integrates nitrification kinetics, accounting for the biological release of protons (H^+) over time to ensure long-term pH stability. The platform operates using a database of common physiologically acidic fertilizers, employing stoichiometric constants and solubility product analysis to minimize the risks of nutrient precipitation and equipment failure. Modern web and mobile programming stacks were utilized for the development.

Results. Featuring synchronized computational engines with offline capabilities and a multilingual interface, AquaTune provides a globally accessible solution for the economic and chemical optimization of tank mixtures. Our results demonstrate that this comprehensive approach not only prevents the costly degradation of chemical components but also enhances the environmental sustainability of plant protection programs. AquaTune emerges as a unique, science-based alternative to traditional volumetric methods, transforming complex chemical equilibrium modeling into an efficient, field-ready decision support tool.

Conclusions. The developed AquaTune application integrates complex chemical models of carbonate equilibrium and nitrification kinetics into a user-friendly interface for precision agriculture. This enables farmers to optimize the composition of working solutions, preventing pesticide degradation and equipment clogging, thereby increasing the efficiency and environmental sustainability of the farm.

Key words: acidity, alkalinity, digital agriculture, pesticide application, plant protection, water quality.

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