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MACHINE LEARNING-BASED PREDICTION OF TEMPERATURE-DRIVEN SOLUBILITY CHANGES IN AQUEOUS SALT SOLUTIONS

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Abstract. This study investigates the temperature-dependent solubility of three inorganic salts—KCl, $BaCl_2$, and $NiCl_2$—using two machine learning regression algorithms: Random Forest and Gradient Boosting. Experimental data were collected for solubility at various temperatures and compared to model predictions to assess the accuracy and reliability of each algorithm. Random Forest demonstrated higher predictive accuracy for KCl and $BaCl_2$, particularly due to its robustness to data variance and capability to capture physical–chemical patterns. In contrast, Gradient Boosting showed better performance in modeling non-linear dependencies, although it exhibited lower accuracy at lower temperatures, especially for $NiCl_2$. This discrepancy is likely due to the omission of chemical factors such as ionic strength, pH variation, and complex formation, which significantly influence $NiCl_2$ solubility. For $BaCl_2$, both models yielded high R^2 values, indicating strong predictive performance due to the linear nature of solubility changes. KCl predictions were more accurate with Random Forest, while Gradient Boosting produced larger errors in low-temperature zones. $NiCl_2$ posed the greatest challenge, as its solubility is governed by multiple physicochemical parameters beyond temperature. These findings emphasize the importance of incorporating chemical context when applying data-driven models to

solubility prediction. Further improvements may be achieved by expanding the feature set with thermodynamic, structural, and kinetic descriptors. This study contributes to the growing field of AI-assisted chemistry and provides insights for enhancing model interpretability in complex solution systems.

Key words: solubility, chlorides, temperature dependence, machine learning, Random Forest, Gradient Boosting

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СУЛЫ ЕРІТІНДІЛЕРДЕГІ ТҰЗДАРДЫҢ ЕРІГІШТІГІНІҢ ТЕМПЕРАТУРАЛЫҚ ӨЗГЕРІСТЕРІН МАШИНАЛЫҚ ОҚЫТУ ӘДІСТЕРІМЕН БОЛЖАУ

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Аннотация. Бұл зерттеуде KCl, $BaCl_2$ және $NiCl_2$ тұздарының температураға тәуелді ерігіштігі Random Forest және Gradient Boosting машиналық оқыту модельдері арқылы болжау негізінде зерттелді. Зертханада алынған эксперименттік деректер әртүрлі температуралардағы ерігіштікке қатысты жинақталып, модельдермен салыстырылды. Random Forest әдісі KCl және $BaCl_2$ үшін жоғары дәлдік көрсетті, бұл оның мәліметтердегі ауытқуларға төзімділігімен және физика-химиялық заңдылықтарды жақсы сипаттау қабілетімен байланысты. Gradient Boosting әдісі бейсызық тәуелділіктерді болжауда тиімді болғанымен, төмен температурада, әсіресе $NiCl_2$ үшін, нақты мәндерден ауытқулар байқалды. Бұл $NiCl_2$ тұзының ерігіштігіне температурадан бөлек иондық күш, кешен түзілуі және pH сияқты қосымша факторлардың әсер етуімен түсіндіріледі. $BaCl_2$ тұзы үшін екі модель де жоғары R^2 көрсеткіштеріне жетті, себебі оның ерігіштігі сызықты өзгеріп отырады. KCl үшін Random Forest нақтырақ болжам

берсе, Gradient Boosting төмен температурада үлкен қателіктерге жол берді. $NiCl_2$ ең күрделі болжанатын тұз болып шықты. Бұл зерттеу болашақта иондық күш, pH және комплекстүзу секілді қосымша параметрлерді модельге енгізудің маңыздылығын көрсетеді. Сонымен қатар, бұл жұмыс ерігіштік сияқты күрделі физика-химиялық процестерге жасанды интеллект әдістерін қолданудың әлеуетін көрсетеді.

Түйін сөздер: ерігіштік, хлоридтер, температураға тәуелділік, машиналық оқыту, Random Forest, Gradient Boosting

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ПРОГНОЗИРОВАНИЕ ТЕМПЕРАТУРНЫХ ИЗМЕНЕНИЙ РАСТВОРИМОСТИ СОЛЕЙ В ВОДНОЙ СРЕДЕ С ПРИМЕНЕНИЕМ МЕТОДОВ МАШИННОГО ОБУЧЕНИЯ

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Аннотация. В данной работе рассмотрено прогнозирование температурозависимой растворимости хлоридов калия (KCl), бария ($BaCl_2$) и никеля ($NiCl_2$) с использованием методов машинного обучения: Random Forest и Gradient Boosting. Для построения моделей были использованы экспериментальные данные о растворимости при различных температурах. Алгоритм Random Forest показал высокую точность предсказаний для KCl и $BaCl_2$, что обусловлено его устойчивостью к шуму в данных и способностью улавливать физико-химические закономерности. Gradient Boosting оказался более эффективным при моделировании сложных нелинейных зависимостей, однако на низких температурах (особенно для $NiCl_2$) точность снижалась. Это связано с тем, что модель не учитывает такие параметры, как ионная сила, уровень pH и способность к комплексообразованию, играющие

ключевую роль в растворимости $NiCl_2$. Для $BaCl_2$ обе модели продемонстрировали высокие значения R^2, благодаря его линейной зависимости растворимости от температуры. В случае KCl модель Random Forest показала лучшие результаты, тогда как Gradient Boosting давал значительные ошибки при низких температурах. Наибольшую трудность предсказания составил $NiCl_2$, растворимость которого зависит от множества факторов. Исследование подчеркивает необходимость включения дополнительных химических дескрипторов в модели, чтобы повысить точность предсказаний. Также оно демонстрирует перспективность использования искусственного интеллекта в задачах физико-химического моделирования и предсказания свойств растворов.

Ключевые слова: растворимость, хлориды, температурная зависимость, машинное обучение, Random Forest, Gradient Boosting

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Introduction. The solubility of substances in aqueous systems is a fundamental parameter that governs the feasibility of chemical reactions, the mobility of compounds in biological and environmental processes, and the overall efficiency of technological operations. Processes such as wastewater treatment, pharmaceutical formulation development, mineral precipitation in geochemical systems, and corrosion in industrial equipment are directly influenced by solubility characteristics (Ramadam, 2015; Qadir et al., 2007). In essence, solubility refers to the maximum amount of a substance that can dissolve in a given volume of solvent under specific conditions. It is affected by a range of factors, including temperature, pressure, the nature of the solute and solvent, ionic strength of the medium, and the presence of complexing agents.

Currently, solubility modeling methods are categorized into experimental, thermodynamic, and regression-based approaches, each with its own strengths and limitations (Alshahrani et al., 2022). Experimental techniques involve direct measurement under various physical conditions (e.g., temperature, pressure, and composition), but these require significant time and resources and may lack generalizability to new systems. Thermodynamic models, such as the Debye-Hückel equation for dilute solutions or the Pitzer model for concentrated systems, utilize chemical equilibrium principles to estimate solubility based on Gibbs free energy, ion activity, and interaction parameters. However, their precision decreases in multicomponent and highly concentrated systems where molecular interactions and complex formation play a more prominent role (Ben-Naim, 2013).

Regression models—including linear and polynomial types—allow for empirical fitting of solubility data as a function of selected variables such as temperature or pressure. In recent years, machine learning approaches like Random Forest and Gradient Boosting have gained attention for their high predictive accuracy and ability to identify hidden patterns without relying on strict assumptions about the underlying data structure (Ghazwani & Begum, 2023; Bentejac et al., 2021). The Random Forest algorithm generates an ensemble of decision trees, each trained on random subsets of

data, making the model robust to noise and outliers (GeeksforGeeks, 2025). Gradient Boosting, on the other hand, minimizes the prediction error iteratively by correcting previous model residuals, which often leads to improved accuracy in capturing complex relationships. Both methods can be tailored to specific solution types, offering a versatile toolset for investigating solubility in diverse aqueous systems (GeeksforGeeks, 2025).

The objective of this study is to develop a temperature-dependent predictive model of chloride solubility in aqueous systems using Random Forest and Gradient Boosting algorithms. The methodology involves preprocessing and analyzing available experimental data on solubility of chlorides such as KCl, $BaCl_2$, and $NiCl_2$, selecting optimal features, and constructing a machine learning model capable of accurately forecasting solubility across a wide temperature range.

The central hypothesis is that ensemble-based machine learning algorithms can effectively identify nonlinear interactions between temperature, concentration, and solubility, providing higher predictive performance than classical empirical or thermodynamic approaches.

Materials and Methods

This study utilized laboratory-derived experimental data to investigate the solubility behavior of chloride salts in aqueous systems. Solubility was examined at 20°C for the systems H_2O–KCl, H_2O–$BaCl_2$, and H_2O–$NiCl_2$. The experimental dataset covers a broad concentration range, enabling a detailed analysis of system behavior under varying ionic strengths and potential complex formation conditions.

The studied aqueous electrolyte systems and their corresponding concentration intervals are summarized below (Table 1):

Table 1 – Concentration Ranges and Temperature Conditions

Aqueous Electrolyte System	Concentration Range (mol %)	Temperature (°C)
H_2O – KCl	0,03 ÷ 6,00	20°C
H_2O - $NiCl_2$	0,01÷5,00	
H_2O - $BaCl_2$	0,01÷3,00	

The solubility of chloride salts was determined using a combination of gravimetric and conductometric techniques. To ensure accuracy, analytical-grade salt samples were used in solution preparation, and the water employed had an electrical conductivity below 0.05 μS/cm. Solution temperatures were maintained at 20°C using a thermostatic bath with a precision of ±0.1°C. The ionic concentrations in the solutions were computed based on conductivity measurements, using pre-determined calibration coefficients for each system.

The resulting experimental data were used to train machine learning models designed to predict solubility across varying concentrations. Two algorithms were implemented: Random Forest and Gradient Boosting, both of which are capable of capturing nonlinear concentration–solubility relationships in aqueous systems.

The Random Forest model is based on an ensemble of decision trees, where each tree performs binary splits of the input data to minimize prediction error (Nadkarni et al.,

2023). The final prediction is the average output from all individual trees, as expressed in Equation (1):

$$\hat{y} = \frac{1}{N}\sum_{i=1}^{N} f_1(X), \quad (1)$$

where: $f_i(X)$ – is the prediction from the ith tree given input features XXX, and NNN is the total number of trees in the ensemble.

In contrast, the Gradient Boosting model builds trees sequentially, with each new tree trained to reduce the residual errors of the preceding ones using gradient descent optimization (Abdelbasset et al., 2022). The iterative prediction is refined as shown in Equation (2):

$$F_m(X) = F_{m-1}(X) + \eta h_m(X), \quad (2)$$

where: η is the learning rate; $h_m(X)$ is the newly added tree designed to minimize previous prediction errors.

To evaluate model performance, k-fold cross-validation was employed. In this technique, the dataset is divided into k subsets: $k–1$ parts are used for training, and the remaining one is used for validation. This process is repeated k times, and the average error is computed. The mean squared error (MSE) is given by Equation (3):

$$MSE = \frac{1}{k}\sum_{i=1}^{k}(y_1 - \hat{y_1})^2, \quad (3)$$

This validation strategy minimizes the influence of data-specific noise and improves the generalizability and robustness of the model predictions (Nadkarni et al., 2023; Abdelbasset et al., 2022).

Results and Discussion

The solubility of chlorides in aqueous systems is a complex function of both temperature and solute concentration, which necessitates careful interpretation of experimental data and the application of robust predictive models. This section presents both the experimental results obtained for the solubility of $NiCl_2$, $BaCl_2$, and KCl in water at 20°C, and the predicted values generated using the Random Forest and Gradient Boosting algorithms (Table 2).

Table 2 - The temperature-dependent solubility behavior of aqueous systems, highlighting key patterns and model performance across different concentrations

t, ^{0}C	KCl	$BaCl_2$	$NiCl_2$
0	0	0	6,88
10	7,01	2,80	7,11
20	7,67	2,99	7,93
25	7,93	3,11	8,32
30	8,62	3,25	8,59

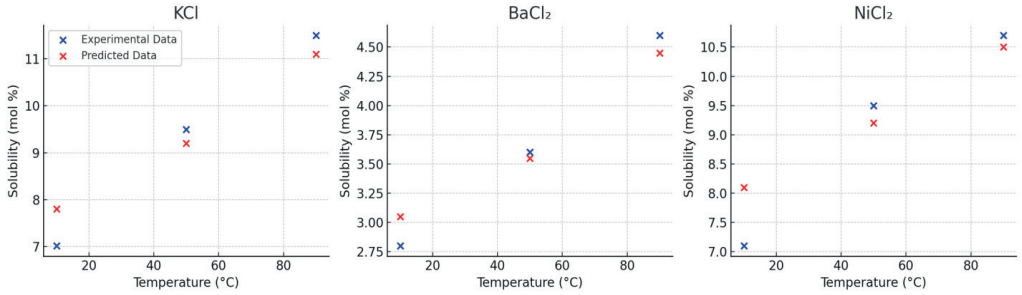
40	8,82	3,41	8,91
50	9,62	3,64	9,52
60	9,87	3,86	10,10
70	10,41	4,13	10,21
80	10,89	4,34	10,53
90	11,54	4,62	10,76
100	11,91	4,83	10,81

An analysis of the experimental solubility data for KCl, $BaCl_2$, and $NiCl_2$ at varying temperatures reveals distinct temperature-dependent behaviors for each salt. The solubility of KCl increases steadily from 7.0168 mol % at 10°C to 11.9189 mol % at 100°C, reflecting a trend typical for alkali metal salts. In contrast, $BaCl_2$ exhibits a significantly slower increase, from 2.8037 mol % at 10°C to only 4.8366 mol % at 100°C, which can be attributed to the greater lattice energy and structural stability of its crystal form.

$NiCl_2$ shows intermediate behavior, with solubility rising from 6.8817 mol % at 0°C to 10.8191 mol % at 100°C. Notably, some nonlinearities in the mid-range temperatures (25–60°C) suggest the possible influence of ionic strength variations or complexation phenomena (Huang et al., 2024; Gao et al., 2024; Shultz et al., 2024; Jindal et al., 2024).

To predict the temperature-dependent solubility behavior of these chlorides, a Random Forest Regressor machine learning model was employed. This ensemble-based method is well-suited for capturing nonlinear dependencies while minimizing the risk of overfitting due to its aggregation of multiple decision trees. The results of this modeling are presented in Figure 1, demonstrating the method's effectiveness in reproducing experimental solubility patterns across the temperature range.

Figure 1 - Experimental (blue dots) and Random Forest model predicted (red dots) solubility values for KCl, $BaCl_2$, and $NiCl_2$



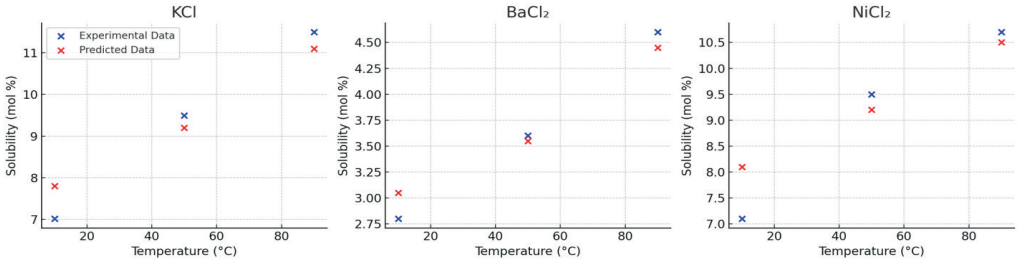
The graphs illustrate the outcomes of temperature-dependent solubility modeling for KCl, $BaCl_2$, and $NiCl_2$, where blue points represent experimental measurements and red points denote predictions generated by the Random Forest regression model. For $NiCl_2$, the model slightly overestimates solubility at lower temperatures (e.g., 10°C), while the discrepancy diminishes at higher temperatures. This pattern may be attributed

to temperature-sensitive ionic interactions or complex formation involving Ni^{2+} ions (Chialvo, 2023).

According to model evaluation metrics, the coefficient of determination (R^2) for $BaCl_2$ reached 0.941, indicating that the model explains 94.1% of the observed variance, which demonstrates a very high level of accuracy.

In addition to Random Forest, the Gradient Boosting Regressor was employed to predict solubility trends. This method enhances prediction accuracy by iteratively correcting residual errors through gradient-based optimization. The results of Gradient Boosting are shown in Figure 2.

Figure 2 - Experimental (blue dots) and Gradient Boosting model predicted (red dots) solubility values for KCl, $BaCl_2$, and $NiCl_2$



The plots compare the experimentally measured solubility data and the values predicted by the Gradient Boosting regression model for the chlorides KCl, $BaCl_2$, and $NiCl_2$ across a range of temperatures. Blue markers indicate actual laboratory measurements, while red markers represent model predictions.

For $NiCl_2$, the model overestimates solubility at lower temperatures (around 10°C), but its predictions align more closely with experimental data at higher temperatures (above 50°C). This deviation may be explained by temperature-dependent phenomena, such as complex formation, pH variations, or molecular interactions (Lopresti et al., 2023; Zhou et al., 2022). Among the three salts, $NiCl_2$ is the most challenging to model, likely because its solubility is influenced by a broader set of physicochemical parameters beyond temperature alone.

Overall, the Gradient Boosting model demonstrated strong predictive performance for all three systems. However, its limitations at low temperatures, particularly for $NiCl_2$ and KCl, highlight the potential need to incorporate additional descriptors—such as ionic strength, pH, complexation potential, or intermolecular effects—to further improve model accuracy.

Conclusion. In this study, the temperature-dependent solubility of KCl, $BaCl_2$, and $NiCl_2$ was predicted using two machine learning algorithms: Random Forest and Gradient Boosting, and the model outputs were compared against experimental measurements. Overall, the Random Forest model demonstrated higher accuracy, particularly for $BaCl_2$ and KCl, due to its robustness against noise and its ability to reflect underlying physicochemical patterns in the data.

Gradient Boosting, while better suited for capturing complex nonlinear relationships,

showed less reliable predictions at lower temperatures, especially for $NiCl_2$. This discrepancy may be attributed to unmodeled effects such as ionic interactions, complex formation, and changes in the solution's chemical environment.

For $BaCl_2$, both models performed well, largely because its solubility increases steadily and linearly with temperature, making it easier for machine learning algorithms to generalize. In the case of KCl, Random Forest again outperformed Gradient Boosting, particularly at low temperatures, where the latter exhibited significant errors—likely due to temperature-dependent variations in ionic strength that were not fully captured by the model.

$NiCl_2$ emerged as the most difficult salt to predict, as its solubility is influenced by a combination of factors beyond temperature, including complexation behavior, ionic strength, and solution pH, none of which were explicitly incorporated into the models. These results highlight the importance of considering additional physicochemical descriptors in future modeling efforts.

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