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Mechanistic Coupling of Coagulation-Flocculation, and Machine Learning for Removal of Various Contaminants from Water System

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Abstract: - Water is the most precious compound on the earth. Presence of different pollutants in water is a major cause of pollution. Numerous materials and technologies have been used to remove these pollutants from the water supply. Access to safe water for everyone is the prime aim of sustainable development goal six. To do this, numerous materials and technologies have been created. Coagulation-flocculation and adsorption are the prime steps for treatment of wastewater. Coagulation-flocculation is done in tandem to counter the stabilizing force present to disturb the suspended particles' impurities and toxic materials, so as to allow collision of particles and lead to growth of flocs. Acute and chronic illnesses in humans can result from heavy metal ion concentrations that are higher than advised. Adsorption is effectively applied techniques for removal of these heavy metals and rest of the materials present in water. Machine learning helps to analyze the contaminants in water to develop a suitable technique and materials for removal of contaminants from water. The aim of this paper is to couple the coagulation-flocculation, and machine learning techniques together for removal of all contaminants from the water system and explain the mechanism which helps to know the chemical interaction.

Keywords: Coagulation, flocculation, mechanism, machine learning, contaminants, water system

1. Introduction

The water related problems are caused by increasing world population which utilizes large amounts of water and produces large amounts of contaminants. In order to minimize the disturbance of ecological balance of the receiving water, it has to undergo treatment before getting released to the environment. The character of wastewater and domestic water is decisive for the selection of a treatment scheme (Koul et al 2022). The previous work reveals that impurities are associated with both suspension and dissolved (Jabin et al 2023). So it is very necessary to understand the details of impurities in domestic water and wastewater. From the standpoint of water engineering, Water is an intricate system that is tainted by a variety of contaminants.

Suspended matter can be both organic and inorganic in nature (Bryukhov et al 2022). The fine fractions of suspended solids carry significantly high pollutant loads as compared to other water pollutants. Thus, high concentration of suspended solids can contribute to various adverse effects such as high turbidity, high total suspended solids (TSS), chemical oxygen demand (COD) and biological oxygen demand (BOD) (Shabanizadeh and Taghavijeloudar, 2023). Turbidity is one of the most unaesthetic parts of any type of water; whether it is industrial water, groundwater or surface water. The variation in the turbidity of water at different levels makes it difficult to handle. Many other pollutants have strong affinity to TSS and therefore such other pollutants present in water are removed with TSS (Kapoor et al 2015). So it is very necessary to study the details of physico-chemical properties of different varieties of water (Kumar et al 2015). The impurities of water are divided in three different categories on the basis of their size (Figure 1 (A)). They may be settleable suspended matter (100 µm), non settleable suspended matter (0.08-100 µm) and dissolved matter (0-0.08 µm) in the water system.

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Ideally, industrial effluent is treated before being discharged into the environment or being used again for any purposes. Industrial wastewater regulation, however, varies by area, with many nations lacking strong legislative frameworks backed by regulatory organizations. More than 60% of industrial effluents in underdeveloped nations have been disposed of untreated, according to UNESCO (The United Nations world water development report 2017). However, enterprises are finding it difficult to comply with the strict water discharge and reuse standards as more nations tighten their regulatory frameworks. The traditional methods of treating wastewater to remove various contaminants have a number of issues, including low removal efficiency, excessive energy consumption, and the production of poisonous sludge (Kumar, and Chawla 2014; Saini et al 2018). In an effort to raise the treated effluent's quality, the researchers have put forth a variety of substitute therapeutic approaches. These consist of membrane separation, electro-technologies, photocatalytic reactions, coagulation-flocculation and adsorption (Saini et al 2019, Chawla et al 2015, Nayyar et al 2022). For the treatment of wastewater contaminated with high quantities of suspended, colloidal and heavy metals, coagulation-flocculation and adsorption are widely employed. Munch et al. in 1980 discussed and summarized the findings of different scientists and classified the contaminants according to their size and the same has been shown in figure 1 (B).

There isn't a thorough and analytical analysis of the literature that addresses the most recent advancements in the removal of dangerous suspended and colloidal particles, heavy metal ions from various wastewater sources with the effective role of machine learning. Thus, the purpose of this work is to study the latest developments in the removal of dangerous suspended and colloidal particles, heavy metal ions from various wastewater sources with the effective role of machine learning.

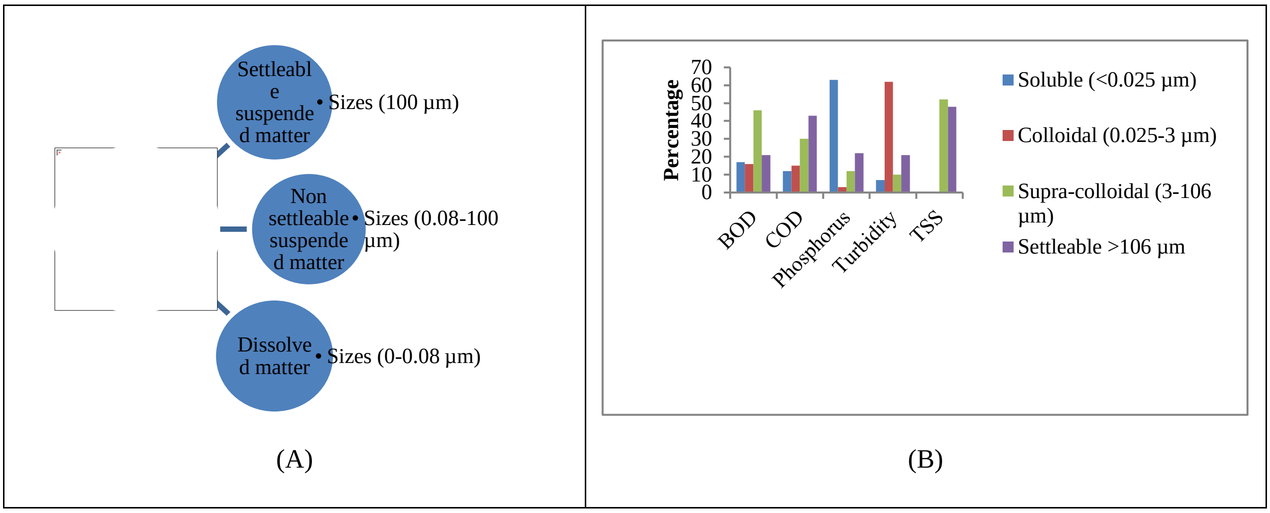

Figure 1: (A) Type of impurities in water and their probable sizes (B) Solubility percentage of BOD, COD, Phosphorus, Turbidity and TSS in water

2. Methodology

In this study the mechanistic role of coagulation-flocculation, adsorption and optimization for removal of various contaminants and heavy metal ions is discussed. This research is split into three primary sections.

A) Coagulation-flocculation mechanism for removal of suspended contaminates

B) Machine learning for water treatment

3. Discussion

3.1 Coagulation-flocculation technique

Coagulation-flocculation is an important physicochemical operation. It is used in the treatment of different kinds of water. This technique is done in tandem to counter the stabilizing force present to disturb the suspended particles, so as to allow collision of particles and lead to growth of flocs. Coagulation and flocculation play an important role in many wastewater treatment schemes (Raj et al 2023). Because of a complex relationship of various parameters in the coagulation-flocculation process, a thorough understanding of these phenomena is important. The goal of coagulation-flocculation is to overcome the force that stabilizes the suspended particles, enabling particle collision and flocculation growth (Brempong et al 2023). The colloid particles have brownian motion in water, so their surfaces are generally negatively charged and they repel each other and form stable and dispersed suspension. The term "floculation" describes the series of collisions that occur in a flocculation basin when destabilized particles are rapidly mixed together by hydraulic shear force (Badawi, et al 2023). The amount of coagulants essential for coagulation is proportional to the concentration of dissolved organic matter present in water. As per literature, the optimization of coagulation-flocculation is the most vital parameter in drinking water and to meet the goal of turbidity removal (Loganathan et al 2020). They stressed the significance of adopting a treatment objective in the coagulation technique and highlighted the necessity of evaluating coagulation as a multiple input process which can be adjusted by two important parameters; pH and coagulant dosage (Kapoor et al 2015). The coagulant dosage depends upon the types of wastewater and pH (Jabin et al 2021). Proper coagulation-flocculation is important for good clarification and filtration performance as also for control of pathogens. Improper coagulation can lead to high coagulant residuals which increases the turbidity of water (Jabin et al 2021).

There is no reliable formula to determine the effective dosage of coagulants and flocculants. However, the jar test is the most consistent technique to determine the effective coagulant-flocculant and its dosage (Kapoor et al 2015). At higher colloidal concentration, destabilization by adsorption and charge neutralization occur early, but continued addition of coagulant results in reversal of charge as well as re-stabilization (Jabin et al 2021). At a very high colloidal concentration, enough colloids should be present for the coagulation-flocculation process. A few literatures reported that high turbid water requires less amount of coagulant/flocculant than water with low turbidity (Jabin et al 2023). In the presence of suspended solids, low molecular mass polymers preferentially reacted with soluble organics, while high molecular mass polymers at low dosage preferentially reacted with suspended solids. At a higher dosage, when the coverage of suspended solids surface by polymer increases, polymers begin to interact with humic substances. The presence of suspended solids brings about an increase in the chances of humic substance removal. Coagulation can be accomplished with a variety of coagulants, some of which have been covered here.

3.1.1 Role of metal coagulants:

The most popular and economical inorganic coagulant is salt of aluminum i.e. alum ($Al_2 (SO_4)_2.nH_2O$), and it is used extensively as an efficient coagulant in water treatment (Hargreaves et al 2018). But a major disadvantage in the use of Al/Fe salts is their instant and uncontrolled hydrolysis and fast precipitation when added to water (Jabin et al 2021). Poly aluminum chloride and ferric chloride have been broadly utilized as inorganic coagulants in water treatment (Rizvi et al 2022). As per previous studies, dosage of coagulant is prime factor (Youssef et al 2023). As per Otálora et al in 2022, iron salt produces heavy floc and removes suspended matter very efficiently (Otálora et al 2022). According to them, salt of iron can be used over a broad range of pH and it can remove turbidity and color from industrial wastewater successfully. As per Kalavathy et al in 2017, a comparable amount of dosage shows greater pH drop in $FeCl_3$ treated water than in alum treated water (Kalavathy et al 2017).

3.1.2 Coagulation mechanism with aluminum salt

Alum is most used inorganic coagulant for wastewater treatment. Destabilization done by charge neutralization of colloidal particles in presence of $Al(OH)_3$ results in formation of sweep floc. The mechanism involved here includes inter particle bridging, charge neutralization and sweep coagulation. The mechanism of coagulation in aluminum salt is controlled by hydrolysis speciation. The positive charged poly-hydroxy complexes like $[Al_8(OH)_{20}]^{+4}$ are effective coagulants in the pH range of 4 - 7 (Malik et al 2018). Alum is a good coagulant in itself which can remove organic matters to a great extent. The quantum of organic matters in water affects the optimum pH for coagulation with alum (Bakar and Halim, 2013). For effective flocculation to take place sufficient amount of alkalinity is needed. Therefore by adjusting coagulant dosage and pH in optimum range alum can prove to be an excellent organic remover (Cruz et al 2020). But in low pH water, low alkalinity inhibits effective $Al(OH)_3$ formation. Organic removal increases with increase in alum dosage. The polymerized alum solution: polyaluminum chloride (PAC), polyaluminum sulphate and polyaluminum chlorosulphate occur with different degrees of polymerization. Polyaluminum chloride (PAC) has been used widely for the last few decades as a coagulant. Sodium aluminate $NaAlO_2$ is having a variety of industrial applications and can be used as a coagulant in drinking water treatment also. It has also been applied in the past to remove phosphate.

3.1.3 Coagulation mechanism with iron salt

The commonly used iron salts are ferric chloride, ferrous sulphate and ferric sulphate. Effective coagulation with iron salts takes place in a similar pH range as that of aluminium salts. The characteristics of flocs formed with iron salt are similar to salts of aluminium (Bakar and Halim, 2013). . Iron salts are usually difficult to dissolve and are corrosive. Effluents carry a large amount of soluble iron concentration if iron salts are used as primary coagulants. Iron salts produce good results when the condition is acidic in nature (Akinnawo et al 2023). As per previous studies, few hydrolysis products of cationic nature are formed and it was concluded that such products interact strongly with negative colloids with correct dosage and pH (Akinnawo et al 2023). Excess dosage results in reversal of charge and colloids get re-stabilized. But iron salts impart color in the effluents when used in high dosage. Ferrous sulfate generally reacts either with added alkalinity or natural alkalinity to form ferrous hydroxide.

The inorganic coagulants usage has its own limitations. A large amount of coagulants is required and subsequently a large volume of sludge is generated (Bakar and Halim, 2013). In contrast, a proper use of polyelectrolytes can successfully remove pollutants from different kinds of wastewater. With the development of the chemical industry, the organic polyelectrolytes were introduced for the treatment of different types of water. Since then polyelectrolytes are being used in water treatment as flocculants. Non-ionic and anionic polyelectrolytes are less toxic, whereas cationic polyelectrolytes have been found to be more toxic particularly to aquatic organisms (Gregory and Barany, 2011). Due to apprehension of toxicity, Japan and Switzerland have prohibited the use of polyelectrolytes as primary coagulants. When polyelectrolyte is used as primary coagulant, it introduces toxicity in water bodies because the dosage of polyelectrolyte is high when it is used. solo in water treatment (Naumenko, 2021). The recommendation of NSF International (National sanitation foundation-2001) for commonly used commercial polyelectrolytes are: < 50 mg/l for polydiallyl dimethyl ammonium chloride, < 20 mg/l for polyamine based polyelectrolytes and 1mg/l for polyacrylamide based polyelectrolytes irrespective of charge density. So to avoid the above problems particularly on a large scale, the only solution is to use polyelectrolytes as a coagulant aid/ flocculants in conjunction with inorganic coagulants (Jabin et al 2023). The benefit of using polyelectrolyte in conjunction with inorganic coagulant is low polyelectrolyte dose, small amount of sludge generation, less ionic load in treated water and reduced dosage of inorganic coagulant (Jabin et al 2023). Chemistry of polyelectrolytes for coagulation-flocculation technique has been discussed in the following section.

3.1.4 Role of polyelectrolytes in coagulation-flocculation

A polyelectrolyte is formed by identical monomers called homo-polymers. More complex macromolecules that consist of more than one monomer are known as copolymers. Water-soluble and having flexible chain structures are the characteristics of the polymers utilized in wastewater and water treatment. These polymers are called polyelectrolytes. The simplest primary structure of such molecules is a linear chain of atoms connected by chemical bonds. It is particularly advantageous in dealing with slow settling flocs in coagulation at low temperature and in treatment of light coloured water where they increase the toughness of flocs and settle ability. Cationic polyelectrolytes are more effective in removal of turbidity and suspension as compared to anionic and non-ionic polyelectrolytes (Jabin et al 2023).

Natural polyelectrolytes have the advantage because they are toxic free even at high dosages (Badawi et al 2023; Deepa et al 2022). Starch behaves like a natural polyelectrolyte. It may be cationic or anionic, or non-ionic in nature, depending on the monomer units (Sibiya et al 2022). The cationic type has quaternary ammonium group substitutions and the anionic type has carboxylic substitutions group (Badawi et al 2023). There are also a few natural anionic polyelectrolytes available. Among all of them, tannin has received attention in wastewater treatment but it is very pH specific (Santos et al 2019). As per literature, the most important natural polyelectrolyte is chitosan (Jagaba et al 2018). It is obtained by partially deacetylated chitin which are copolymers of N-acetyl-α-D- glucosamine and α-D- glucosamine (Jagaba et al 2018). It is having medium molecular weight. But high molecular weight is essential when reaction is carried out by a bridging mechanism. Long chain polymers attach on a few sites on a particle leaving long loops and tails which stretch into the surrounding water (Jagaba et al 2018). Starch, a polymer can be converted to cationic polyelectrolyte by combining with primary –OH group in alkali treated starch along with N-trimethyl ammonium chloride so that cationic portion is attached through ether link to the polymer chain (Sibiya et al 2022). Few lignin based flocculating agents have been found in literature (Wu et al 2022). They are prepared and modified by kraft lignin to provide them cationic character. Anionic polyelectrolytes with low or medium charge density and high molecular weight are more appropriate for flocs (Guan et al 2021). If too many polyelectrolytes are used then the whole particle surface gets coated with polyelectrolytes and no site will be available for bridging. Large flocs are formed with the help of cationic polyelectrolyte when the coagulated solids have a slightly negative charge. A few non ionic polyelectrolytes have also received attention in water treatment. They include starches, cellulose derivatives, gelatins and glues (Sibiya et al 2022). They are used as flocculants in solid-liquid separations. They vary in structure and molecular weight. They are easily acceptable because of biodegradable nature, although natural polyelectrolytes have the advantage of being free of toxicity (El-taweel et al 2023).

But synthetic polyelectrolytes are more widely used as they are more effective as flocculants due to the possibility of controlling properties; such as molecular weight, number and type of charge units and others (Jabin et al 2023). Molecular weight and charge density of a polyelectrolyte generally affect the destabilization mechanism and result in floc formation (Jabin et al 2021). The intensity of charge carried by the polyelectrolyte depends upon the degree of ionization of the functional groups, or on the degree of copolymerization or substitutions (El-taweel et al 2023). Functional groups along the polyelectrolyte chain, besides the possibility of carrying a charge, are also sites which possess the property of being adsorbed. Therefore, it is understandable that destabilization by polyelectrolytes could involve a mechanism combining both charge neutralization and effects due to adsorption. Polyelectrolytes are effective in enhancing the orthokinetic flocculation rate when added to a system already destabilized with metal coagulants.

As per literature, polyelectrolytes are also used as primary coagulants, replacing the need of metal coagulants (Jabin et al 2021). Polyelectrolytes are used significantly as primary coagulants in many cases to minimize turbidity of surface waters. Some literature concluded that cationic polyelectrolytes (poly diallyl dimethyl ammonium chloride) are efficient to replace inorganic coagulants successfully for high as well as low turbid waters (Ma et al 2018). Literature also shows that polyelectrolytes are also capable of removing organic colors (Ishak et al 2020). By testing a variety of commercially available cationic polyelectrolytes and exploring their effectiveness in precipitating fulvic acid, it was observed that the polyelectrolytes vary in their efficiency to minimize organic colors. Polyelectrolytes have been studied by several researchers in the destabilization and minimization of microorganisms in wastewater (Ishak et al 2020) In addition, cationic polyelectrolytes are more effective in destabilization whereas anionic polyelectrolytes generally produce inferior results in removal of microorganisms (Ma et al 2018).

Polyelectrolytes are also used as flocculant aids in both wastewater and municipal water treatment (Verma et al 2016). Further, they are added with metal coagulants to get the desired result (Jabin et al 2023; Su 2023). The aim of using polyelectrolytes as secondary coagulants is not only for destabilization but also supplementing the orthokinetic process and changing properties of floc in terms of increasing floe size, compressibility, density, shear strength, permeability, and settleability. It could be observed from literature that best results are found when polyelectrolyte is added after the addition of metal coagulant (Gregory et al 2011; El-taweel et al 2023). There are few cases where particles and polyelectrolyte are of opposite sign, polyelectrolyte addition before metal coagulant could serve to reduce the surface charge of particles on adsorption thereby subsequently reducing the quantity of metal coagulant required to effect charge reduction (El-taweel et al 2023). It has also been found that metal coagulants do not always reduce polyelectrolyte dosage since they function (Sun et al 2021). Dosage of the polyelectrolyte is the most deciding factor for coagulation-flocculation technique (Sun et al 2021). Excess dose of coagulant and flocculant leads to restabilization. Cationic polyelectrolytes are found to be more effective as primary coagulants as per literature.

3.1.5 Flocculation mechanism of polyelectrolytes

The flocculation mechanism of particles can be broadly divided into two categories: polymer bridging and charge neutralization.

(A) **Bridging mechanism**

A small dosage of long chain polymers added to a suspension of colloidal particles adsorb on to them in such a way that each chain gets attached to two or more particles forming a bridge as shown in Figure 2(A). This mechanism is called polymer bridging. Interestingly, flocculation by bridging takes place up to a certain dosage of polymer only, which starts diminishing thereafter (Zhou et al 2021; El-taweel et al 2023). This phenomenon is called steric stabilization. The fundamental requirement for polymer bridging to start is that there has to be enough vacant space on particles surface so that chains of polymer segments get attached to the particles and that the span of each pair of particles should be such as to promote inter particle repulsion (Dayarathne et al 2021). On the other hand adsorbed amount should not be too high, otherwise particle surface will be completely covered and insufficient adsorption site will be available. In this case, particles get re-stablize (Figure 2 (B)). The aggregates (flocs) formed by bridge flocculation is much stronger as compared to the ones formed by the addition of salts (Zhou et al 2021; El-taweel et al 2023). Whereas, under high shear strain such stronger flocs are produced by the bridging mechanism but if it is broken, it may not re-form again.

(B) Charge neutralization

The bridge mechanism helps to understand the effects of nonionic and anionic polymers on the flocculation of colloidal particles. However, it has been observed that in case of flocculants with high cationic charges in anionic colloidal suspensions, the involvement of high energy of attraction supports a flattened adsorbed surface which considerably diminishes the chance of formation of loops and trains to bridge the suspended particles (Guan et al 2021). In this circumstance, each charged location on the particle's surface cannot be neutralized by an oppositely charged polymer segment due to geometric restriction, which results in polymer chains to adsorb to produce “patches” of charge surrounded by areas of opposite charge. This gives rise to strong attraction between oppositely charged adsorbed patches and surrounded areas (Figure 2 (C)).

It is evident from above that at low particle concentration with high cationic charge on the flocculants and anionic colloidal solids, charge neutralization would prevail. However, at high particle concentration for collisions to take place on a time scale similar to the one required for the polymer to attain a flattened configuration, bridging mechanism would be predominant. Therefore, the controlling mechanism of flocculation is determined by flocculants concentration.

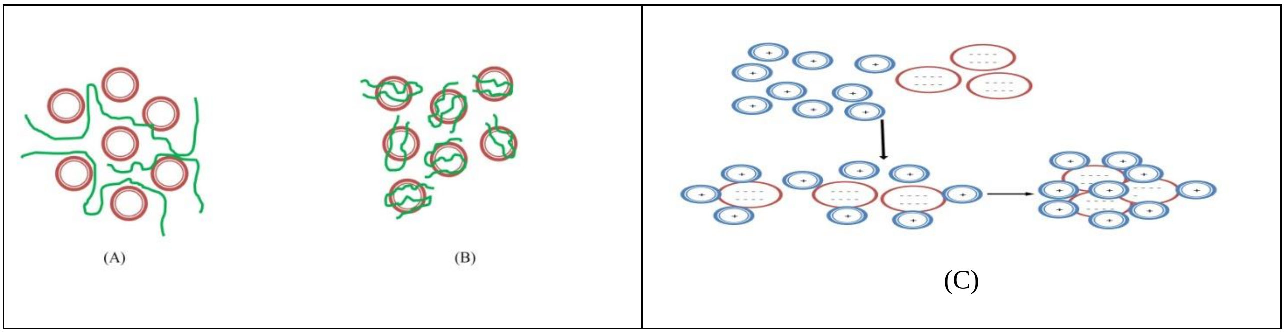

Figure 2: Schematic diagram of (A) Polymer bridging (B) Restabilzation by adsorbed polymer chain (C) Charge neutralization for flocculation

Dosing and mixing prominently affects the level of flocculation. It has been found that flocculation takes place rapidly at high solid concentration and low polymer dosage, but the flocs so formed are not stable and get broken even at moderate stirring. So the floc size (and settling rate) can be kept at peak levels without subsequent decline by reducing the rate of stirring shortly after polymer dosing. This is however, extremely difficult in practice due to precise control required. It has been observed that optimum flocculation takes place when half the area is covered with polyelectrolytes. As the concentration increases from this level, the degree of flocculation decreases as the particles may be completely covered by the adsorbed polymer layer (El-taweel et al 2023). Therefore overdosing may result in creation of a well established suspension, which is not desirable. However in principle a sufficient level of flocculation can be achieved with much lower polymer dosage.

3.2 Machine learning for water treatment

These days, machine learning (ML) approaches are among the most popular engineering tools because of their many benefits, one of which is their ongoing improvement. Noticeable progress in fields such as mathematics, neurology, engineering, psychology and economics along with advances in processing speed of computer systems set the stage for the emergence of the first wave of artificial intelligence. The advent of the “Big Data” term in the 21st century led to the second wave of AI. This wave introduced statistical models trained on "Big Data." These models lacked the contextual properties but had good classification and prediction abilities. Statistical models have become popular because of the significant development of machine learning and including deep learning techniques. Machine learning models create a mathematical model based on "training data". The model is then tested for accuracy by feeding with testing data. Deep learning, which is a subset of machine learning, works efficiently with unstructured or unlabeled data. In recent years, research has gained momentum in the field of prediction of water system. The challenge in dealing with water related data lies in: nonlinearity and variability caused by human interference and changes in climatic conditions which are unpredictable. AI models especially deep learning models have gained success in handling such nonlinear data (Safeer et al. 2022).

Artificial intelligence's machine learning (ML) branch focuses on creating and analyzing statistical algorithms that can learn from data, generalize to new data, and carry out tasks without explicit instructions. To forecast probable contamination occurrences, artificial intelligence (AI) algorithms can examine past data on pollution sources and water quality. Authorities can reduce hazards and protect water resources by being proactive in spotting patterns and trends. By evaluating large, complicated data sets to identify the most practical and economical treatment options, artificial intelligence (AI) can optimize water treatment procedures. This optimization may result in less energy and chemical use, which would ultimately lessen the environmental impact as a whole. Water samples with particular contaminants can be promptly identified using AI-driven image recognition and pattern recognition technology. This aids in customizing the purification procedure to effectively eliminate the detected contaminants. AI can help research and development teams uncover novel materials and technology for water treatment more quickly. Prior to carrying out actual trials, machine learning can assist in identifying potential solutions and simulating their efficacy (Figure 3)

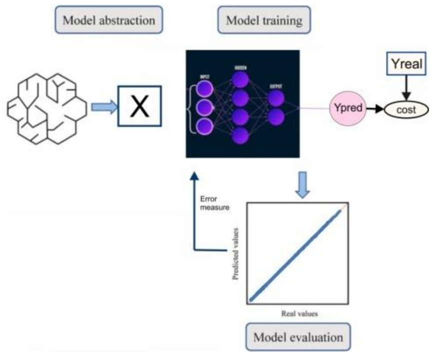

Figure 3: The working of ANN model

The use of AI in water quality and purification systems is not without its difficulties, though. A few of the issues that need to be resolved are data security, privacy, and the requirement for qualified workers to oversee and understand AI systems. In general, the incorporation of AI into water quality and purification systems has the potential to greatly enhance water management, rendering it more effective, sustainable, and adaptable to the increasing worldwide water shortages. These AI algorithms can be applied in various areas like waste management (Kumari et al. 2023), wastewater treatment (Alam et al. 2022), reuse of waste material, resource extraction (Pandey et al. 2023) etc. Artificial Intelligence models can simulate the targeted pollutants' removal.

In a wastewater treatment, coagulation is a crucial stage. The jar-test method, zeta potential measurements, artificial intelligence techniques (including neural networks, fuzzy and expert systems), and combinations of these techniques are currently employed in the water industry to help operators and engineers in the water treatment process determine the optimal dosage of the coagulant. Jar tests are used to calculate the necessary coagulant dose, but they take a while to complete and don't react instantly to variations in raw water quality that occur during the day. In order to get around this restriction, the researchers created artificial neural network (ANN) models. They did this by using full-scale wastewater treatment plant data, which was used to calibrate the model and estimate the coagulant dose while taking raw water into account as an input and adhering to treated water quality characteristics. With a correlation coefficient of 0.872 and a mean squared error of 0.016, the best model could forecast the coagulant dosage (Tochio). The process of determining the appropriate dosage of coagulant for water treatment is a laborious one that involves multiple parameters and nonlinear data correlations. To calculate coagulant dosage, a graph attention multivariate time series forecasting (GAMTF) model was created and compared to deep learning and traditional machine learning methods by Lin et al. 2023. The GAMTF model performed better than the other models (R2 = 0.63 - 0.89, RMSE = 4.80 - 38.98), accurately predicting settling water turbidity and coagulant dosage at the same time. By taking into account the underlying links between characteristics and their previous states, the GAMTF model increased prediction accuracy.

Random Forest (RF), Artificial Neural Networks (ANN), Linear Regression (LR), Simple LR, Gaussian method, Decision Stump method, Quinlan's M5 algorithm with regression function (M5P), Smola and Scholkopf's Sequential Minimal Optimization algorithm with LR (SMOreg), and the Adaptive Neuro-Fuzzy Inference System (ANFIS) techniques have been compared by Arab et al 2022 for sustainable operation of coagulation and flocculation process. Additionally, Central Composite Design created the experimental data using the Response Surface Methodology (CCD-RSM) in order to optimize the system. The elimination of turbidity is mostly influenced by two factors: slow mixing speed and $FeCl_3$ dosage, with P-values of less than 0.0001 and 0.005, respectively. The results of this study demonstrate that, under ideal circumstances, CCD-RSM can forecast a maximum removal efficiency of 92%. Furthermore, the ANFIS and RF models have demonstrated the best accuracy levels in eliminating water turbidity, with R^2 values of 0.96 and 0.92. In conclusion, a Petri-Net model creates a Conceptual model to perform managerial insights for water treatments in an intelligent manner.

AI models in predicting the doses of coagulants and biopolymers in coagulation–flocculation processes for the treatment wastewater have been widely investigated by researcher (Matovelle et al. 2023). The leachates generated in sanitary landfills contain many pollutants harmful to the environment (Durai et al. 2020; Mishra et al. 2018). The researchers have used Artificial Neural Networks (ANNs) to determine the doses of coagulants and biopolymers suitable for coagulation–flocculation processes. An Artificial Neural Network model attempts to mimic the working of neurons that make up a human brain. As shown in Figure 5, the ANN consists of three layers, Input Layer: it accepts inputs that can be different formats provided by the programmer. Hidden Layer: The performs all the calculations to find hidden features and patterns. Output Layer: The hidden layer performs various transformations on Input layer, finally resulting in output which is conveyed using this layer. The use of ANNs reduced the number of operations of the tests of jars in the laboratory, hence optimizing the resources. The ANN model was fed with the real dataset of the results obtained related to the effectiveness of applying biopolymers in leachate treatments at different concentration levels. The model verified that the applied coagulation–flocculation treatments helped in reducing the turbidity values in the leachate and other contaminants associated with suspended solids. This helped in optimizing the jar tests which in turn reduced the operational costs.

Abdi, and Mazloom 2022 studied the capacity of several cutting-edge and reliable machine learning (ML) techniques, such as Random Forest, Extreme Gradient Boosting, Light Gradient Boosting Machine (Light GBM), and Gradient Boosting Decision Tree, to forecast the adsorptive removal of penta-valent arsenate ions from wastewater across 13 distinct using metal organic frameworks (MOFs). A number of statistical criteria were used to assess the produced models. The results showed that the Light GBM model, which has R2, RMSE, STD, and AAPRE (%) of 0.9958, 2.0688, 0.0628, and 2.88, respectively, offered the best accurate and dependable response to predict penta-valent arsenate adsorption by MOFs. The Light GBM model reasonably anticipated the expected trends of penta-valent arsenate elimination with increasing starting concentration, solution pH, temperature, and coexistence of anions. Sensitivity study showed that the adsorption process is directly dependent on the dosage and surface area of MOFs and has an undesirable relationship with the starting penta-valent arsenate concentration

Aftab et al 2022 have studied the role of machine learning for adsorption of multi- metal using bio-adsorbents. Bio-adsorbent is a dry weight ratio of mandarin peel, maple leaves, and tea waste of 3:2:1. Model creation uses two machine learning techniques: artificial neural networks (ANN) and support vector regression (SVR).

Additionally, the same set of data is used with the widely used multiple linear regression (MLR) technique. The coefficient of determination (R2), mean relative error (MRE), root mean square error (RMSE), and average absolute relative error (AARE) are statistical evaluation measures used for model evaluation. The R2 values obtained for SVR models are 0.9981, 0.997, 0.998, and 0.997, respectively, whereas the created MLR models for cadmium, copper, lead, and zinc have R2 values of 0.831, 0.8676, 0.8739, and 0.8567, respectively. The values of this parameter for the ANN models developed for each of the aforementioned metals in that order are 0.0901, 0.0911, 0.0683, and 0.2069, respectively. The values of this parameter AARE calculated for the SVR models for the four different metals (Cd, Cu, Pb, and Zn) are 0.0586, 0.102, 0.063, and 0.176, respectively. SVR and ANN models are among the most accurate and widely applicable machine learning methods. The breakthrough curves predicted by the SVR and ANN models closely resemble the experimental curves when the input parameters are changed, while the breakthrough curves projected by the MLR models significantly deviate from the experimental values.

Conclusion

Coagulation-flocculation, and machine learning techniques are effectively applied for treatment of water. Suspended, colloidal and other dissolved impurities and toxic chemicals are effectively precipitated out using coagulation-flocculation methods. However, the rest of the toxic heavy metal ions and other contaminants are effectively removed by adsorption methods. Machine learning also played a crucial role for treatment of water. Machine learning is effectively applied to analyze the contaminants in the water system. Continuous assessments of these contaminants in the water system through machine learning helped to develop the methods and technologies for the removal of these contaminants from the water system. A smart soft sensor predicts and controls the coagulation and flocculation process using a variety of machine learning methods. Because of its complicated and non-linear behavior, coagulation and flocculation process are challenging to optimize and anticipate. Consequently, using ML computations is an appropriate way to get around this obstacle. But one of the problems with ML research is that there isn't enough data, which we solve by utilizing an eight-year archive of experiments. This work demonstrates that machine learning techniques can handle complex challenges involving big datasets and can serve as cost-effective substitutes for costly and labor-intensive experimental wastewater treatment procedures. This paper also explains the mechanistic steps of coagulation-flocculation and role of machine learning for removal of contaminants.

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