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Article

Analysis of nanomaterial-enhanced concrete durability and explore its biomechanical implications based on molecular dynamics simulation

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Abstract: The purpose of this paper is to analyze the influence, application potential and biomechanical significance of nano-materials on the durability of concrete by means of molecular dynamics simulation. In this study, the whale optimization algorithm-back propagation neural network (WOA-BPNN) model was used to predict and optimize the optimal content of different nano-additives in concrete. The results show that these nano-materials can effectively reduce the chloride diffusion coefficient of concrete and improve its impermeability and durability, among which nano-silica is the most outstanding. By discussing the action mechanism of nano-materials, it is found that they can penetrate into the microstructure of concrete, reduce pores, enhance compactness, and improve the chemical stability of concrete through chemical reactions. Although the application of nano-materials faces challenges in cost, dispersion and stability, it shows great potential in improving the durability and biomechanical properties of concrete, which provides a new way for the modification and optimization of concrete materials. The research results play an important role in promoting the application of nano-materials in concrete field and improving the safety and service life of building structures.

Keywords: nano-materials; concrete; durability; biomechanics; molecular dynamics simulation; whale optimization algorithm-back propagation neural network (WOA-BPNN)

1. Introduction

In the field of modern architecture, due to the low cost, high compressive strength, and abundant raw materials, concrete is used as a kind of building material. Concrete is one of the most important structural materials, and its performance and durability are directly related to the safety, stability and service life of buildings. The durability of traditional concrete materials is often difficult to meet the needs of long-term use when faced with multiple factors such as extreme environment, chemical erosion and physical wear [1]. Based on this reason, exploring new concrete modification technology and improving its durability has become one of the hot spots in the current scientific research of building materials [2]. With its unique physical and chemical properties, nano-materials show great potential in improving the microstructure of concrete, enhancing mechanical properties and improving durability [3]. By adding nanoparticles to concrete, the pore structure can be refined, the density can be improved, and the interface bonding force can be enhanced, so as to improve the impermeability, frost resistance and chemical erosion resistance of concrete to a certain extent [4]. The appearance of this technology will not only open up a new way for improving the performance of concrete materials, but also provide the possibility for prolonging the service life of buildings and reducing maintenance costs.

The application of nano-materials in concrete is not always smooth. How to choose the appropriate nano-materials, determine the reasonable dosage and optimize the proportion scheme to achieve the best modification effect is an important challenge facing the current research [5,6]. Although the traditional test method can directly reflect the performance changes of materials, it is often time-consuming, laborious and expensive, and it is difficult to fully consider various influencing factors [7]. Based on this reason, it is the key to solve this problem to establish an efficient and accurate prediction model with the help of modern intelligent algorithms [8]. As a new swarm intelligence optimization algorithm, WOA has been widely used in function optimization, machine learning, data mining and other fields because of its simplicity, easy realization and strong global search ability [9–11]. BPNN is a classical neural network model, and the nonlinear mapping from input to output is realized by adjusting the network weights with the help of back propagation algorithm [12]. Nano-materials can penetrate into the microstructure of concrete because of its extremely small particle size and high specific surface area, and significantly improve the compactness, chemical stability and durability of concrete through filling effect, chemical reaction and interface enhancement. Compared with traditional concrete materials, nano-modified concrete shows superior performance in dealing with extreme environment, chemical erosion and physical wear, which is of great significance for prolonging the service life of building structures and reducing maintenance costs. Combining WOA with BPNN can make full use of WOA's global search ability to optimize the network structure and parameters of BPNN, so as to improve the prediction accuracy and generalization ability of the model.

Based on this idea, the purpose of this study is to build a prediction model of reinforced concrete durability based on WOA-BPNN. By collecting a large number of experimental data, the model is trained and verified to ensure the accuracy and reliability of its prediction performance. Then, the model is used to predict the durability of concrete with different nano-materials, and the influence law of nano-material types and content on the durability of concrete is analyzed, which provides scientific basis for the design, application, and Its Biomechanical Implications of nano-modified concrete. The purpose of this study is to explore the influence of this new biomaterial (nano-material reinforced concrete) on specific mechanical properties of cells, including cell morphology, adhesion and migration ability, in order to provide scientific basis for improving the biomechanical properties of concrete materials.

The significance of this study lies in:

(1) With the introduction of nano-materials and intelligent algorithms, it provides a novel perspective for the modification of concrete materials, aiming at promoting the continuous progress of concrete science.

(2) A prediction model based on WOA-BPNN is established in this study. The model can comprehensively consider various influencing factors and realize accurate prediction of concrete durability.

(3) By combining model prediction with experimental verification, this study explores the internal mechanism of nano-materials to improve the durability of concrete, which provides a basis for scientific and reasonable selection of

nano-materials and determination of their proportions.

(4) By improving the durability of concrete materials, this study is helpful to significantly extend the service life of buildings, thus reducing resource consumption and environmental pollution.

2. Summary of related theoretical basis

2.1. The core connotation of concrete durability

The durability of concrete, as a key index to measure its long-term service performance, covers the ability to resist physical erosion, chemical corrosion, biodegradation and mechanical damage [13]. It involves many dimensions such as impermeability, freeze-thaw cycle, chemical erosion resistance, carbonation resistance and crack resistance. For example, the carbonization of concrete will lead to steel corrosion, which will also affect the durability of reinforced concrete structures. Impermeability is also related to the resistance of concrete to moisture and gas penetration. The freeze-thaw cycle tests its stability in cold environment [14]. Concrete structures in cold regions are usually affected by freeze-thaw cycles (FTCs), this will lead to the premature failure of concrete structures. Additionally, salt solutions, for example, sulfate ions and chloride ions in saline soil or coastal regions will also corrode concrete structures. Thus, chemical corrosion resistance requires that concrete can resist the destruction of corrosive media such as acid, alkali and salt. Anti-carbonation is related to the maintenance of the internal alkaline environment of concrete [15]. Crack resistance is directly related to the integrity and long-term stability of concrete structures. These properties together constitute a comprehensive assessment system of concrete durability, which is the key to ensure the safety and durability of building structures.

2.2. Innovative application of nano-materials in concrete modification

Nano-materials, with their unique nano-scale size effect and surface effect, quantic effects and the greater surface-area-to-volume ratio, have brought unprecedented opportunities for the modification of concrete materials. Nanomaterials are characterized as sheets, cylinders, and spheres. At present, it has shown obvious benefits in building materials. It is a kind of new synthetic material to combine concrete with nanomaterials. Compared to conventional concrete, it will show superior mechanical properties. Nanoparticles can penetrate into the microstructure of concrete, and improve the compactness and mechanical properties of concrete by filling pores, enhancing interface bonding and promoting hydration reaction [16]. For example, nano-SiO_2 (NS), has been characterized to have a small particle size, strong surface adsorption, large specific surface area, and high surface energy. And the addition of nano-silica and nano-alumina can not only refine the pore structure of concrete and improve its impermeability, but also enhance the mechanical properties and durability of concrete to a certain extent [17]. However, the application of nano-materials also faces some problems, such as high cost, poor dispersibility and compatibility challenge with concrete matrix. For this reason, how to select nano-materials scientifically and reasonably, optimize their dosage and dispersion technology to achieve the best modification effect has become a hot and difficult point in current research.

2.3. Fusion framework of WOA and BPNN

In order to cope with the complexity and nonlinearity in concrete durability prediction, the fusion model of WOA and BPNN is introduced in this study. WOA has realized efficient search and optimization on a global scale by simulating the stages of contraction and encirclement, hunting prey and bubble net attack during whale foraging [18]. With its powerful nonlinear mapping ability and self-learning ability, BPNN has shown remarkable advantages in dealing with complex nonlinear problems [19].

Whale, as a giant in the ocean, is not only one of the most spectacular creatures in nature, but also the largest animal category on earth. Mature whales can reach 30 meters long and weigh more than 180 tons, showing the amazing vitality and adaptability of nature. The whale family is huge, including seven main species: killer whales, minke whales, plug whales, humpback whales, right whales, fin whales and blue whales, each of which plays an indispensable role in the marine ecosystem. As mammals that need to rise to the surface to breathe regularly, whales have developed a unique sleep mode-hemispheric sleep, in which one side of the brain stays awake to control breathing, while the other side enters a rest state.

The bubble net predation strategy adopted by humpback whales is particularly unique, which has become an important source of WOA inspiration in this study. Humpback whales can swim around the school of fish skillfully, and form a bubble curtain by releasing bubbles, trapping their prey in it and then hunting. **Figure 1** vividly depicts the scene of humpback whales implementing bubble net predation strategy.

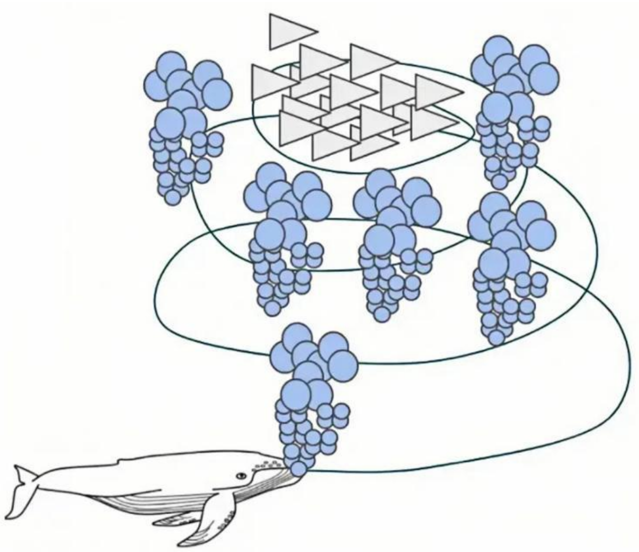

Figure 1. Bubble-net feeding.

In the WOA-BPNN fusion model, WOA is used to optimize the network structure parameters of BPNN, including weight and bias, in order to find the global optimal solution. This fusion will not only give full play to WOA's global search ability, but also make full use of BPNN's local optimization and generalization ability. With the help of iterative optimization, the model can more accurately capture the complex relationship between concrete durability influencing factors and performance, and provide strong support for accurate prediction of concrete durability.

3. Concrete durability prediction model based on molecular dynamics simulation

There are many factors affecting the durability of concrete, including the nature of raw materials, mix design, construction conditions, environmental factors and service history [20]. Data preprocessing first involves cleaning the original data to remove the adverse effects such as abnormal values and missing values. Then, according to the nature of the data, normalization or standardization is carried out to eliminate the differences between data of different dimensions. Finally, according to the specific needs of model input, the data is scientifically and reasonably divided into training set, verification set and test set, which are used for model training, verification and performance assessment respectively. In order to ensure the same thickness of the protective layer around the reinforced concrete, the reinforced concrete specimen shown in **Figure 2** was prepared by vertically placing the rebar with the diameter of 10 mm and the length of 100 mm in the middle of the specimen.

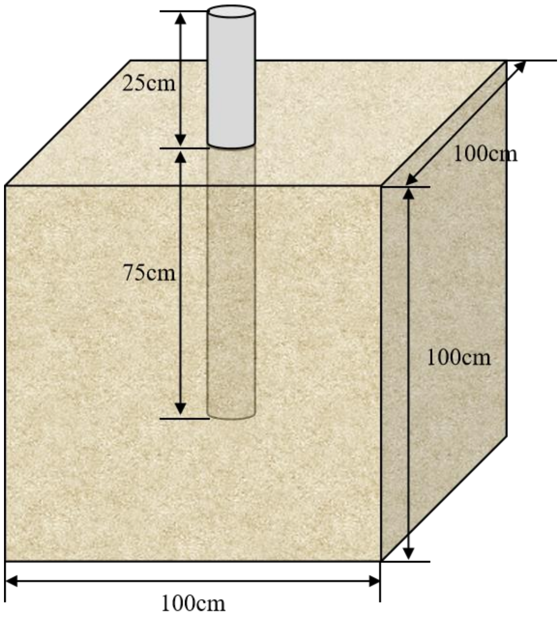

Figure 2. Reinforced concrete specimen.

After the specimen is molded for 24 h, the mold is removed, and the exposed steel bars are wound with copper wires to facilitate electrification, and then epoxy resin is applied to prevent the exposed steel bars from rusting during curing. After 28 days of standard curing, the experiment of electrification in saline soil environment was carried out.

WOA is a swarm intelligence optimization algorithm that simulates the whale's foraging behavior. It realizes the global search of the problem space by simulating the whale's search, encirclement and predation process in the ocean [21]. In WOA, whale individuals gradually approach the global optimal solution by constantly adjusting their positions [22]. BPNN adjusts the network weight by means of back propagation algorithm, and realizes the nonlinear mapping from input to output. In BPNN, the input layer is responsible for receiving external information, the hidden layer is responsible for extracting features and the output layer is responsible for giving prediction results [23]. By constantly adjusting the network weight and bias, BPNN can gradually approach the complex nonlinear function and realize the accurate prediction of concrete durability [24]. The structure of BPNN model is shown in **Figure 3**, and WOA optimization model is adopted.

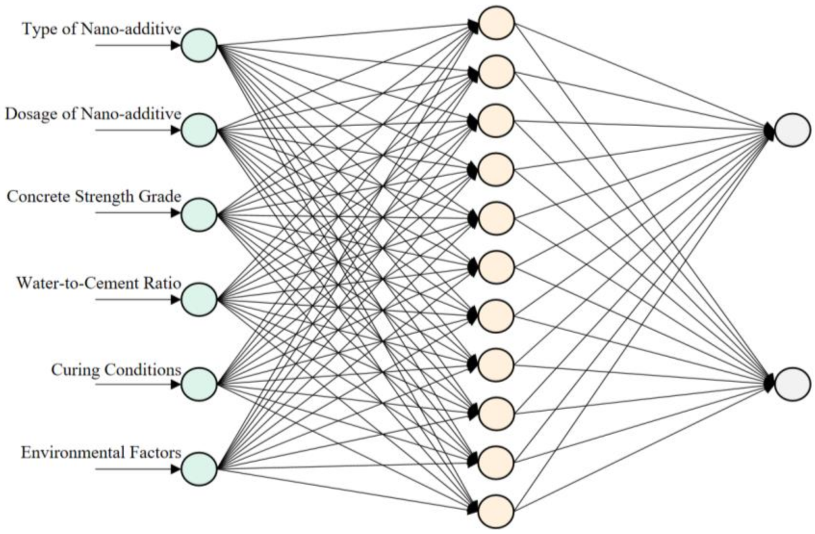

Figure 3. BP neural network structure.

In order to build a concrete durability prediction model based on Whale Optimization Algorithm-Back Propagation Neural Network (WOA-BPNN), the basic structure of the neural network is first defined. According to the number of nodes in input layer, hidden layer and output layer, the structural parameters of the network are determined. Assuming that there are m nodes in the input layer, n nodes in the hidden layer and p nodes in the output layer, the weights and offsets of the network can be expressed as W_{hm} and b_h (hidden layer weights and offsets) and W_{hm} and b_o (output layer weights and offsets).

WOA algorithm is used to optimize the initial weight and bias of neural network. The location update formula in WOA algorithm is as follows:

$$X_{new} = X_{old} + A \times \Delta X \quad (1)$$

where X_{new} is the new position of the whale, representing the parameter update of the neural network, and A is the convergence factor determined by the following formula:

$$A = 2 \times a \times (1 - a)^n \quad (2)$$

In this way, the search range is adjusted in the iterative process to ensure that the algorithm can effectively converge to the optimal solution.

Next, define the output formula of BPNN and describe the process of input signal passing through the network:

$$O = \sigma(W \times X + b) \tag{3}$$

Here, O is the network output, σ is the activation function, and the Sigmoid function is selected:

$$\sigma(z) = \frac{1}{1 + e^{-z}} \tag{4}$$

This function converts linear combination into nonlinear output, which increases the processing capacity of the network.

In order to train the network, it is needed to calculate the output error and adjust the weight and bias accordingly:

$$E = \frac{1}{2}\sum_{i=1}^{p}(O_i - T_i)^2 \tag{5}$$

where E is the network output error, O_i is the actual output of the network, and T_i is the target output.

According to error back propagation, the updating formulas of weight and offset are as follows:

$$W_{new} = W_{old} - \alpha\frac{\partial E}{\partial W} \tag{6}$$

$$b_{new} = b_{old} - \alpha\frac{\partial E}{\partial b} \tag{7}$$

Here, α is the learning rate, which controls the step size of parameter updating.

In WOA algorithm, the strategy of surrounding prey and spiral position update is used to further optimize the network parameters. The formula for surrounding prey is:

$$X_{new} = X_{best} - A \times |X_{rand} - X_{best}| \tag{8}$$

The formula for updating the spiral position is:

$$X_{new} = X_1 + \frac{X_2 - X_1}{2} + \lambda \times L \times cos(2\pi k) \tag{9}$$

Through the above methods, the algorithm can strike a balance between global search and local development.

Using chloride diffusion coefficient D_{Cl} as assessment index to evaluate the durability of concrete:

$$D_{Cl} = \frac{C_s - C_t}{t} \tag{10}$$

By substituting the chloride ion concentration C_t predicted by neural network into this formula, the predicted durability index is obtained, and then the long-term performance of concrete is evaluated.

In the process of model design, some key parameters need to be considered, such as the number of iterations of WOA, population size, search space range, and the learning rate, momentum term and activation function of BPNN.

In the training process, the model is iteratively trained by using the training set data, and the prediction result of the model is gradually close to the actual value by constantly adjusting the network weight and bias. After repeated training and verification, the concrete durability prediction model based on WOA-BPNN is finally obtained. The model can comprehensively consider various influencing factors and realize accurate prediction of concrete durability.

4. Model assessment and performance analysis

After constructing the concrete durability prediction model based on WOA-BPNN, it is particularly important to evaluate its performance comprehensively and objectively. In the preparation stage of new nano-reinforced concrete, the required cement, aggregate and nano-additives are weighed and mixed evenly according to the established ratio. Subsequently, the standard concrete mixing process is adopted to ensure that all components are fully integrated to form a uniform concrete mixture.

For the curing of concrete samples, the temperature and humidity conditions are strictly controlled. The sample is placed in a standard curing room, with the temperature kept at a constant 20 ± 2 ℃ and the relative humidity kept above 95%, so as to ensure the normal hardening and strength development of the concrete sample.

Finally, the WOA-BPNN model and the traditional BPNN model are comprehensively compared and evaluated through multi-dimensional performance indicators such as prediction accuracy, recall, root mean square error (RMSE) and mean absolute error (MAE). As shown in **Figure 4**, the WOA-BPNN model shows significant advantages in prediction accuracy. This is due to the optimization and adjustment of BPNN network structure and parameters by WOA algorithm, which makes the model closer to the actual concrete durability change law. However, the traditional BPNN model is easy to fall into the local optimal solution because it only relies on the gradient descent method for local search, resulting in relatively low prediction accuracy.

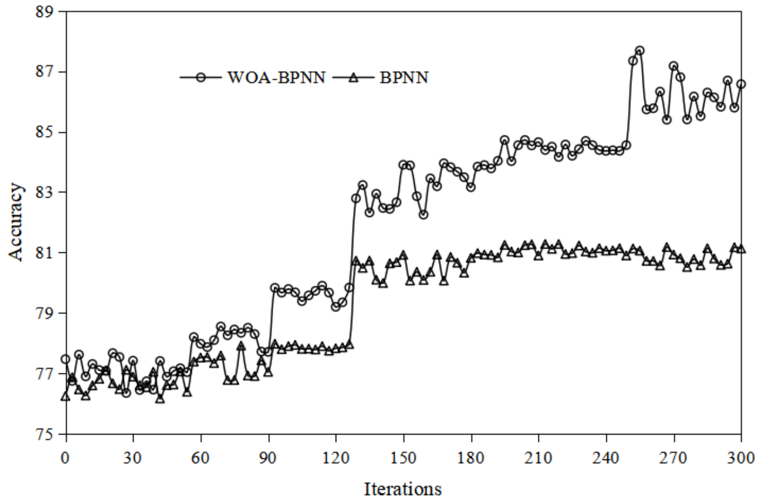

Figure 4. Accuracy comparison.

In the prediction of concrete durability, high recall means that the model can identify the samples with poor durability more accurately. As shown in **Figure 5**, WOA-BPNN model also shows better performance than traditional BPNN model in recall rate. This fully proves that WOA algorithm can not only improve the prediction accuracy, but also enhance the model's ability to identify abnormal or edge situations when optimizing the BPNN model.

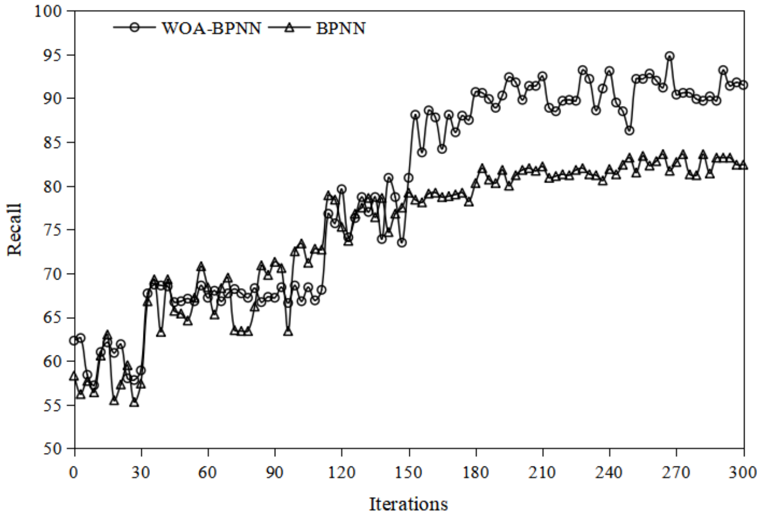

Figure 5. Comparison of recall.

As shown in **Figure 6**, the WOA-BPNN model shows a lower value on the root mean square error (RMSE) index, which shows that the deviation between the predicted result and the actual value is smaller and the prediction accuracy is higher. This result once again verifies the feasibility of WOA algorithm in optimizing the parameters of BPNN model to a certain extent, and the superiority of WOA-BPNN model in concrete durability prediction.

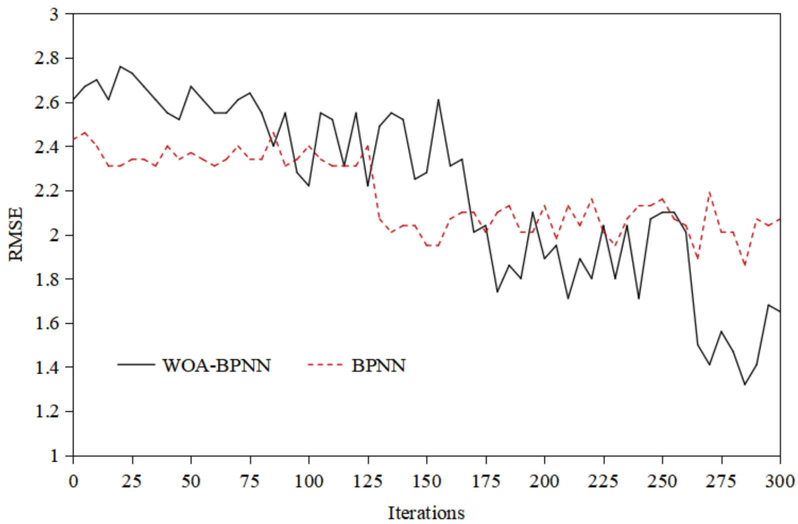

Figure 6. RMSE comparison.

As shown in **Figure 7**, the WOA-BPNN model has also achieved a lower value in the (MAE) index, which fully proves its high accuracy and stability in the prediction of concrete durability. Compared with RMSE, MAE is less sensitive to outliers and pays more attention to the average level of overall prediction deviation.

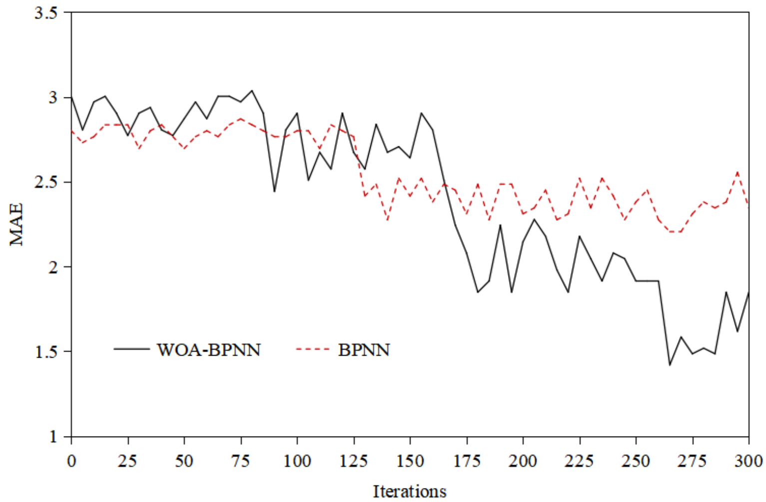

Figure 7. MAE comparison.

With the help of the comparative assessment of multi-dimensional performance indicators such as prediction accuracy, recall, RMSE and MAE, it can be seen that WOA-BPNN model has significant advantages over traditional BPNN model in concrete durability prediction. This will not only be reflected in the improvement of prediction accuracy, but also in the enhancement of the ability to identify abnormal or edge situations and the improvement of prediction stability. These advantages are due to the synergistic effect produced by the combination of the global optimization ability of WOA algorithm and the nonlinear mapping ability of BPNN model.

5. Molecular dynamics simulation of the influence of nano-materials on the durability of concrete

In this study, three representative nano-additives, namely Nano-SiO_2, Nano-Al_2O_3 and Nano-$CaCO_3$, were selected, and five blending gradients from 0% to 7% were set to cover the possible blending range in practical application. The types and dosage configurations of nano-materials are shown in **Table 1**.

Table 1. Types and dosages of nano-materials.

Nano-material	**Dosage Gradients (%)**
Nano-Silica (SiO_2)	0, 1, 3, 5, 7
Nano-Alumina (Al_2O_3)	0, 1, 3, 5, 7
Nano-Calcium Carbonate ($CaCO_3$)	0, 1, 3, 5, 7

Next, the constructed WOA-BPNN model will be used to predict the durability of concrete samples with different nano-materials and dosages, with a focus on the variation of chloride ion diffusion coefficient. The predicted results are summarized in **Tables 2–4**.

Table 2. Effect of nano-silica on chloride diffusion coefficient of concrete.

Dosage (%)	**Chloride Diffusion Coefficient (× 10^{-12} m^2/s)**	**Change (%)**
0	5.68	-
1	4.92	−13.4
3	3.87	−31.9
5	3.21	−43.5
7	2.98	−47.5

Table 3. Effect of nano-alumina on chloride diffusion coefficient of concrete.

Dosage (%)	**Chloride Diffusion Coefficient (× 10^{-12} m^2/s)**	**Change (%)**
0	5.68	-
1	5.01	−11.8
3	4.15	−27.0
5	3.68	−35.2
7	3.42	−39.8

Table 4. Effect of nano-calcium carbonate on chloride diffusion coefficient of concrete.

0	**Chloride Diffusion Coefficient (× 10^{-12} m^2/s)**	**Change (%)**
1	5.68	-
3	5.30	−6.7
5	4.65	−18.2
7	4.05	−28.7
0	3.78	−33.4

With the gradual increase of nano-materials, the addition of all types of nano-materials reduces the chloride diffusion coefficient of concrete to some extent. This shows that its resistance to chloride ion penetration has been improved, and the durability of concrete has been enhanced. Nano-silica shows the best improvement effect at all tested dosages, and its maximum decrease is close to 47.5%. This shows its potential in improving the durability of concrete. Nano-alumina and nano-calcium carbonate, although less effective, also achieved a reduction of nearly 40% and 33% respectively. This proves that they can improve the microstructure and impermeability of concrete to a certain extent.

Nano-materials can improve the durability of concrete, mainly due to its unique physical and chemical properties, such as filling effect brought by high specific surface area, chemical reaction with concrete components and interface strengthening. These mechanisms work together to reduce the pore structure in concrete to some extent and enhance the overall performance of the material. The influence of new biomaterials on the mechanical properties of cells may be related to their nanostructures. Nano-additives can penetrate into the microstructure of concrete, reduce pores and enhance compactness, thus changing the physical and chemical properties of concrete surface. These changes may promote the interaction between cells and the surface of materials and enhance the adhesion and migration ability of cells. In addition, the chemical stability of nanomaterials may also have a positive impact on cell growth and differentiation.

6. Discussion

As the basic material of modern architecture, the durability of concrete is directly related to the safety and service life of the structure. Nanotechnology has shown great potential in improving the durability of concrete because of its unique physical and chemical properties. This paper focuses on the application of nano-materials in improving the durability of concrete, and discusses the influence of nano-materials such as nano-silica, nano-alumina and nano-calcium carbonate on the durability of concrete with the help of WOA-BPNN model.

Nano-materials can penetrate into the microstructure of concrete because of its extremely small particle size and high specific surface area, and significantly reduce the pores and micro-cracks in concrete through the filling effect, thus enhancing the compactness and impermeability of materials. Nano-materials can also react with calcium hydroxide and other components in concrete to generate more stable compounds, thus comprehensively improving the chemical stability and durability of concrete.

In this study, nano-silica, nano-alumina and nano-calcium carbonate all show the effect of improving the durability of concrete. Because of its excellent filling effect and chemical reactivity, nano-silica achieved the maximum reduction of chloride diffusion coefficient at all tested doses, showing the best potential in improving the durability of concrete. Although the effects of nano-alumina and nano-calcium carbonate are slightly inferior, they have also made significant improvements.

The action mechanism of different nano-materials may be different, so in practical application, it is necessary to choose the appropriate nano-materials and their dosage according to the specific engineering requirements and concrete performance requirements. For example, for concrete structures that need high impermeability and chemical stability, nano-silica may be a better choice; However, nano-alumina or nano-calcium carbonate may be more suitable when specific mechanical properties and cost control are needed.

7. Conclusions

This study focuses on the application and exploration of nano-materials in improving the durability of concrete and exploring its biomechanical significance. Based on the prediction of WOA-BPNN model, the effects of different nano-additives such as nano-silica, nano-alumina and nano-calcium carbonate on the durability of concrete are analyzed. The results show that these nano-materials can reduce the chloride diffusion coefficient of concrete to some extent and improve its impermeability and durability. Nano-silica showed the best improvement effect at all tested doses, which provided strong support for the modification of concrete materials.

Through comparative analysis, it is found that nano-materials can penetrate into the microstructure of concrete by virtue of their unique physical and chemical properties, reduce pores, enhance compactness, and generate stable compounds through chemical reactions, thus improving the chemical stability of concrete more comprehensively.

The addition of nano-materials also improves the interface structure of concrete and enhances its overall mechanical properties, which is very important for the biomechanical properties of concrete. However, the application of nano-materials also faces challenges in cost, dispersion and stability. Future research needs to explore the composite effect of nano-materials more comprehensively and optimize the dosage configuration to reduce the production cost and improve the application effect.

Ethical approval: Not applicable.

Conflict of interest: The author declares no conflict of interest.

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