

Machine Learning Approaches to Simulate and Predict Packing Density

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Machine Learning Approaches to Simulate and Predict Packing Density

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Abstract

Wet packing density of cementitious material is an important factor determines the performance of concrete. Traditionally, to get the value wet packing density, a large number of experiments must conduct which is time-consuming and labour-intensive. Although there are some empirical models available to calculate the approximate value of wet packing density. But all existing empirical models such as Kwan's model do not consider all the variables that may affect wet packing density, and thus the prediction results of wet packing density are inaccurate when data without considering the variables appear. This research focus on using Artificial Neural Network (ANN) to predict the wet packing density and explore its feasibility and accuracy. After training, the ANN model can give accurate prediction results of wet packing density on most test data, with an overall accuracy of 90.07%. However, there is a certain amount of 'abnormal data' in the data used for training and testing, which seriously affects the training process of the ANN model. It directly leads to the wet packing density values in some prediction results too small or even zero. Overall, the performance of the ANN model is satisfactory and demonstrates the feasibility of using machine learning approach to predict wet packing density, but there is still huge room for improvement.



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1. Introduction

Cement is an important and indispensable building material in modern construction. Therefore, researchers and practitioners in engineering fields need to understand the factors that can affect the performance of the cement. In this project, the wet packing density of cementitious materials is further predicted using a completely new methodology. The wet packing density of cementitious materials can directly affect the flowability of the cement paste, which it further affects the workability and the performance of concrete (Wong & Kwan, 2008). Therefore, obtaining accurate values of wet packing density and optimising its measurement as well as prediction methods are extremely important in modern cement and concrete design.

At present, in order to get the exact value of wet packing density of cement materials, researchers can only carry out a large number of experimental tests. Typically, these experimental tests and measurements are labour-intensive and time-consuming. At the same time, wet packing density depends on many factors, and the experiment's workload increases significantly when more factors are involved. Moreover, the current models and empirical formulas for predicting wet packing density do not take into account the full range of factors, which leads to their inability to predict the exact value of wet packing density and give potentially misleading results to researchers and cement manufacturers.

In order to compensate for the shortcomings and deficiencies of the existing models and formulas, machine learning is used to predict the values of wet packing density. Neural networks are well suited for predicting the value of wet packing density because they do not rely on a large number of empirical formulas and field experimental tests, but only need to use the results of experiments done by researchers in the past to train the model to quickly obtain accurate and reliable prediction of the value of wet packing density.

The purpose of this report is to explore the methodology and its feasibility of machine learning models instead of traditional experimental methods for predicting wet packing density of cementitious materials. This model can significantly reduce the experimental workload and improve the efficiency of cement material and concrete mix design.



2. Literature review

2.1 Packing density of cementitious paste and concrete

From the experimental research conducted by Professor Albert Kwan and Henry Wong in 2007 and 2008, the wet packing density is defined as the maximum solid concentration of cementitious materials under wet conditions (Wong & Kwan, 2008). In a study published by Kwan and Wong in 2008, it was pointed out that higher packing density corresponds to smaller void content, which allows more excess water to act as a lubricant and improve the performance of flowability of cement paste (Wong & Kwan, 2008). Therefore, the packing density of cementitious materials directly affects the flowability of cement paste. At the same time, the flowability of cement paste is a key factor in determining the strength, workability and overall performance of concrete (Wong & Kwan, 2008). In another word, the packing density directly affects the performance of concrete. Therefore, wet packing density plays a critical role in optimising concrete design.

Kwan's research team developed a new method to measure the packing density of cementitious materials, which is called the wet packing method. In this method, water and cement are mixed to change the water/cementitious materials (W/CM) ratio, and the packing density of the cementitious material is defined by the value of solid concentration reaching its peak (Wong & Kwan, 2007).

Kwan's team tested the wet packing method by measuring the packing density of cementitious material containing ordinary Portland cement (OPC), pulverised fuel ash (PFA) and condensed silica fume (CSF). There are three main series of experimental data used to measure the packing density. The first is the cement that contains only one of the OPC, PFA, CSF. A total number of nine tests have been conducted in this series, namely as series 1 (full table in appendix A.1) (Wong & Kwan, 2007). The second is a cement that contains two of the materials from the OPC, PFA, and CSF, a total number of 15 tests have been conducted in the second series, namely as series 2 (full table in appendix A.2) (Wong & Kwan, 2007). The last is cement materials containing all of OPC, PFA and CSF, a total number of ten tests have been conducted in this series, namely as series 3 (full table in appendix A.3) (Wong & Kwan, 2007). In summary, Kwan's team did a total of 34 sets of tests in order to get the



packing density of cementitious materials. Therefore, in order to obtain accurate wet packing density results, a large number of experiments had to be completed.

2.2 Limitations of existing experimental research and model

As mentioned in the previous section, there are only three cementitious materials, which are OPC, PFA, and CSF. In order to get the exact packing density value of cement, Kwan's team did 34 sets of tests using the wet packing method. If there are more types of cementitious materials involved, the number of experimental tests will increase significantly. The existing models used to predict the packing densities of cementitious material are tested by Du and his team. These three models are de Larrard's model, Yu's model and Kwan's model (Du, Li, Pei, & Ma, 2021) (Wong & Kwan, 2014). However, all models only considered a limited number of independent variables, the wet packing density depends on a variety of factors such as water ratio, type of cementitious material, filler and type of superplasticizer used (Du, Li, Pei, & Ma, 2021) (Wong & Kwan, 2008). For example, Kwan's three-parameter model includes the wedging effects and improves the accuracy of the predicted value of packing density, within a 3.55% error (Wong & Kwan, 2014). However, this model does not include the effect of water and chemicals (water-reducing admixture), leading to an underestimation of the packing density result (Wong & Kwan, 2014) (Du, Li, Pei, & Ma, 2021). Therefore, it is very hard to compose a reasonably accurate empirical equation for predicting the wet packing density without testing numerous concrete and/or cementitious pastes with a broad range of all related parameters.

2.3 Machine learning approach

Machine learning is a new technology that has gradually matured and attracted attention in recent years. Its powerful data analysis, processing and prediction capabilities make it widely used in many fields and play an important role in these fields. Machine learning can be categorised into a number of different learning methods, the three most basic and common of which are supervised learning, unsupervised learning and reinforcement learning (Maleki, et al., 2020). Each machine learning method has its own training method and is suitable for different types of tasks.



The first method is called supervised learning, as the name suggests, this type of algorithm requires supervision. The training process involves using data that already contains labels, and the model learns the relationship between the inputs and the corresponding output or results, training the model continuously and eventually achieving prediction or classification of new data (Dongare, Kharde, & Kachare, 2012) (Maleki, et al., 2020). As articulated in Maleki et al's report, the objective of supervised learning is to use many different inputs to predict one or more outputs (Maleki, et al., 2020). Supervised learning can be used on classification and regression problems. For example, the model can be trained by feeding it a large number of pictures of dogs and telling it the breed of the corresponding dog in the picture, which is used to establish the mapping relationship. The model can then be given some brand-new pictures of dog and asked to predict the dog's breed (Barreto & Aibin, 2025). This is an example of classification problem since the dog breeds is a discrete variable and can be classified into different category. Another type of problem is called regression problem, which the output given by the model are arbitrary real numbers rather than a single category (Barreto & Aibin, 2025). For example, consider the data contains information about a large number of vehicles, each with a different brand, year of manufacture, model and other characteristics with their current market value. This dataset can be used to train the model to predict the current value of vehicles. The model can then be given some brand-new information of vehicles and asked to predict the current value of the vehicles (Barreto & Aibin, 2025). This is an example of regression problem because the outputs is the value of vehicle, which is a real number instead of a category.

The second method is called unsupervised learning. Unlike supervised learning, the output of unsupervised learning model is in the form of clusters, patterns or association rules (Subasi, 2020). The main difference between supervised learning and unsupervised learning is that the unsupervised learning model is trained with dataset that does not have any label yet (Barreto & Aibin, 2025). The goal of unsupervised learning is to discover patterns and association from data itself. For example, the company wants to improve the effectiveness of their adverts. By training unsupervised learning model, it categorises customers based on age, geographic location, search habits, gender and previous shopping habits to improve the effectiveness of the ads. Therefore, if a new customer appears in the future, the model will



automatically categorise them to deliver advertisements that are of interest to the customer to maximise the effectiveness of the advertisement (Yadav, 2024).

The last method is called reinforcement learning. Reinforcement learning is thought of in a completely different way from the first two. Reinforcement learning is a form of learning based on 'trial and error' and 'reward mechanisms' (Dongare, Kharde, & Kachare, 2012). The learning model, also called a learner, needs to interact with the environment while correct actions are rewarded, and incorrect actions are punished (Dongare, Kharde, & Kachare, 2012). This will continue and correct its actions to avoid punishment. In other words, the parameter is always adjusting to maximise the reward the learner can be received (Subasi, 2020).

A visualised diagram of three different types of machine learning sees Figure 1 below.

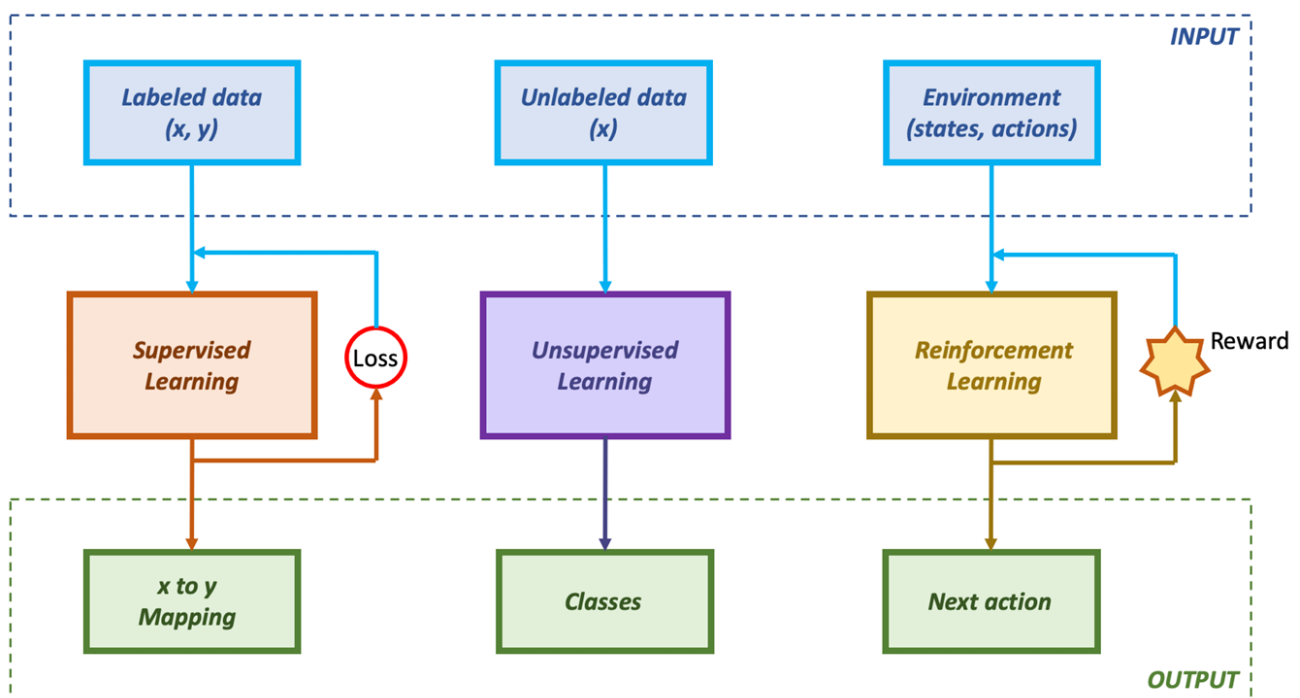


Figure 1 Three different types of machine learning (Giuliano & Innocenti, 2023)

In this project, the goal is to predict the wet packing density of cementitious materials based on past experimental data. In the past experimental dataset, the wet packing density is determined by 37 factors. The factors include SSFA content, SSFA content, RS content, IS content, QS content, FA content, SF content, GGBFS content, WGP content, WGS content,



RA, RFA, Cao content, MgO content, water-cement-ratio, water, cement, Fly ash, silica fume, GGBFS, WGP, RA, RFA, natural sand, Iron sand, Granite (5-10 mm), Granite (10-20 mm), SSFA (5-20 mm), SSFA (≤ 5 mm), QS, Cao, MgO, SP (%), SP (kg), Dosage and void ratio. The corresponding the value of wet packing density as prediction target, full dataset see Appendix B. Since the input to the learning model is all factors mentioned above, and the expected outputs of the machine learning model is the value of wet packing density, which is an arbitrary real number. So, this dataset already contains labels and is a regression problem. Therefore, supervised learning is the most suitable machine learning methods to be used in this project.

There are various approaches to solving regression problems using supervised learning methods. The current approaches are Linear Regression, Decision Trees, Random Forest and Artificial Neural Networks (ANN) (Maleki, et al., 2020). The most basic approach is linear regression, it assumes a linear relationship between the input and output values and trains the model with this assumption (Maleki, et al., 2020). However, in this project, the relationship between wet packing density and input values is not linear. If linear regression model is used in this project, the model's prediction and performance is not optimal. So linear regression model is not adopted. The second approach is called decision trees, it constantly divides the data into different blocks and makes predictions in the corresponding blocks (Rokach & Maimon, 2005). However, the data in the dataset is incomplete, with some experiments recording only a few data and values of wet packing density. The decision tree model can easily overfit and will get a poor performance on predicting the value of wet packing density. So, decision tree model is not adopted. The third approach is called random forest, the random forest model combines multiple decision trees and produce a better prediction than decision tree model [Dutta, Paul, Kumar, 2021]. However, the random forest model is generally computationally expensive, time-consuming and can easily overfitted (Kundu, 2022). Therefore, the use of random forest model is not the best option for this project. The last approach is called Artificial Neural Networks (ANN), ANN as a powerful machine learning tool, are used to model complex, nonlinear relationships. Supervised learning is a training method to identify a relation between the provided inputs and the output result, as highlighted by Dongare et al (Dongare, Kharde, & Kachare, 2012). If there's a difference/error between



the predicted output and the desired value, this error will be reported back to the ANN model and adjusted in the next training process, and this step will loop until the error value is reduced to an acceptable range (Dongare, Kharde, & Kachare, 2012). The ANN does not rely on empirical formulas for wet packing densities and can give accurate predictions taking all factors into account. So, the use of ANN with adequate testing data to obtain on wet packing density of concrete/cementitious paste could give a more accurate prediction and assist the researchers and concrete manufacturers the better understanding the effects of various mix design factors on the performance attributes of concrete without the need of deriving many empirical design equations for different cases of concrete mix design scenarios. Compared with other approaches, ANN is more flexible and have the ability to do parallel processing, which means it can handle multiple tasks at the same time (Mijwil, 2021). Therefore, the use of ANN is well-suited for predicting wet packing densities of cementitious materials.

3. Methodology

The unit used to process information is called a neurone or node in ANN. The ANN contains a large number of nodes that are interconnected by edges in different layer. There are three



main layers, the first one is called the input layer, the second one is called the hidden layers, and the last one is called the output layer.

A visualised diagram of ANN model sees Figure 2.

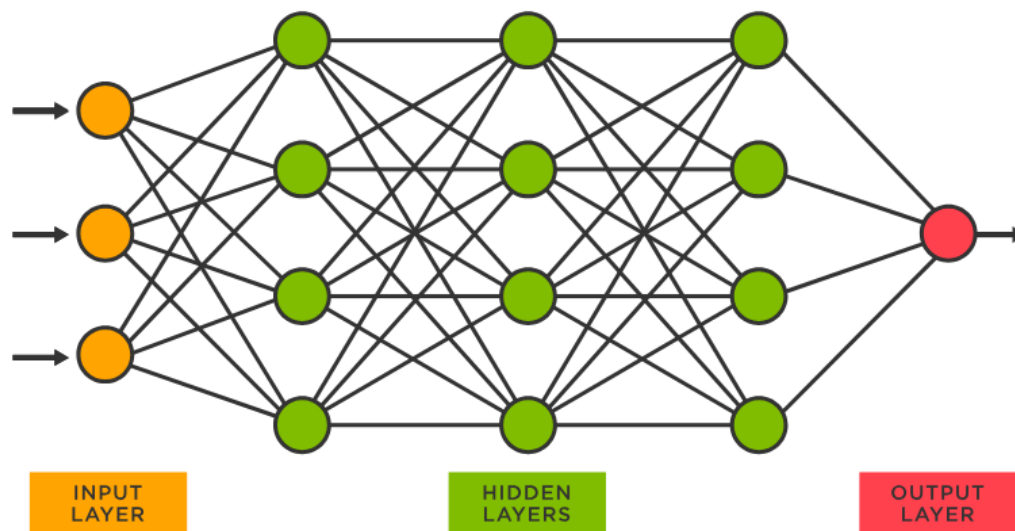


Figure 2 ANN network (Spotfire, 2025)

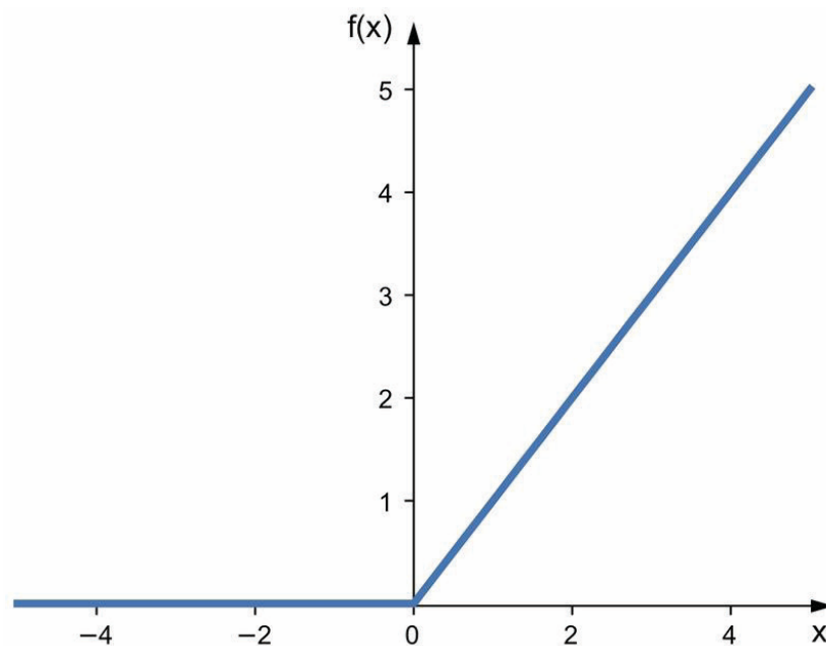


Figure 3 ReLU function (ırmak, 2021)



Firstly, in the input layer, there are 37 nodes and each node represent one of the 37 factors that determines the value of wet packing density. Then the data is transmitted through an edge to the nodes in the hidden layer. Secondly, the nodes can be activated by the activation function in each layer (Dongare, Kharde, & Kachare, 2012). Some popular activation functions includes sigmoid function, identity function, hyperbolic tangent function and ReLU function. All activation functions are all non-linear, which can let the network learn complex patterns (Antoniadis, 2025) (Yadav, 2024). The sigmoid and hyperbolic tangent functions are used in classification problem, while ReLU function is suitable for regression problem. ReLU function is chosen as the activation function used in the hidden layer because the ReLU function is the only one of three functions do not have a computational inefficiency (Dubey, Singh, & Chaudhuri, 2022). A diagram of the ReLU function is shown in Figure 3. The final choice of activation function used in the hidden layer needs to give the closest predicted value to the experimental data. To decide the number of layers and number of nodes in the hidden layer, use Python to continuously test and adjust the number of layers and nodes until the error between real value of wet packing density and predicted value of wet packing density is minimised. After testing, the model's performance is optimal when there are three hidden layers, where the first hidden layer has 64 nodes, the second layer has 32 nodes, and the third layer has 16 nodes. At last, the output layer gives the predicted output from the model. In this project is the wet packing density of cementitious material. From the dataset, the wet packing density is an arbitrary real number. In another word, the predicted output is a continuous variable which means it is a regression problem. As mentioned earlier, ReLU function is the only activation function among the three functions that solves the regression problem. At the same time, it can be noted that the value of wet packing density predicted by the model also has to be a non-negative number, which perfectly fits the range of ReLU function. Therefore, ReLU function is used as the activation function in the output layer.

In the process of training ANN, underfitting and overfitting are two major potential problems that must be taken into account. First of all, underfitting issue means the model has not yet found the relationship between input values and output values, and at this point, when predicting output values using unseen data to test the performance of the model, the error between the real output and predicted output will be very large. Secondly, the overfitting issue



represents the model performs well on the training data. However, if there is unseen data, the poor performance of model due to the model not being generalised to other datasets (Lin, 2020). To avoid the underfitting and overfitting issues, the entire dataset is divided into three parts. The first 60% of the total dataset is used to train the model, the second 20% of the total dataset is used to validate the training model and the last 20% of the total dataset is used to test the training model, this method is called cross-validation and has become an important step in preventing overfitting issue.

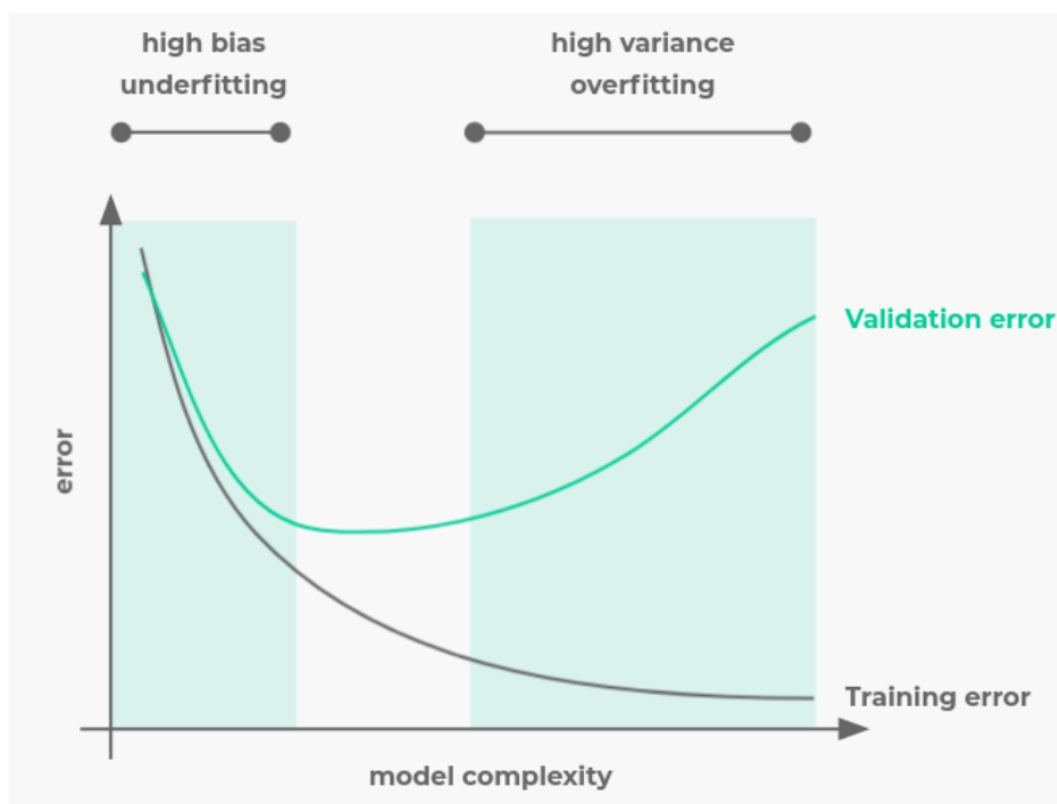


Figure 4 Example of 'Training and validation loss curve' (Sánchez, 2021)

Another purpose of splitting data is to illustrate when underfitting and overfitting issues happen. The underfitting and overfitting issues can be detected by the 'Training and Validation Loss' graph. The horizontal axis is called 'epoch', which represents the number of passes the dataset has been trained and parameter adjusted (mljourney, 2025). The vertical axis is called 'error' or 'loss', which indicates the difference between real value and predicted value. In the graph, the error between the test data's value and predicted value is named as 'training loss', and the error between the validation data's value and predicted value is named



as 'validation loss'. By observing the training loss and validation loss curves, the performance of the model at different epochs can be deduced. An example of 'Training and Validation Loss' graph is shown in Figure 4. From Figure 4, it can be seen that the training error and validation error have high error values when the epoch is small. The green shaded area on the left side of the Figure 4 represents the scenario where the model underfitting problem occurs. As the number of epochs increases, the training error gradually decreases but the validation error keeps increasing. The green shaded area on the right side of the Figure 4 represents the scenario where the model overfitting issue occurs. Therefore, in order to avoid underfitting and overfitting problems, it is crucial to choose a suitable number of epochs, which is the area in the middle of the Figure 4 that is not covered by the shade. Therefore, in order to determine the final number of epochs, it is necessary to repeatedly test different epochs in Python and draw the corresponding training and validation error graphs. At a certain epoch value, if the training error and validation error curves continue to decrease as the epoch increases, and the validation error does not increase, then this epoch value is selected to train the model.

The original data contains experimental data from different researchers. Each researcher conducted different experiments, which means they recorded different variables that determine wet packing density. As a result, there are a lot of gaps in the data. These gaps represent that the corresponding researchers did not consider these variables that would affect the final wet packing density value in their experiments. In order to avoid the problem of skipping a large amount of incomplete data during model training, all blank data are replaced with 0 so that all data can be used to train the model and reduce the time spent on training.

4. Results and discussion

4.1 Results and model performance

The training of model is completed in Python. After repeated and uninterrupted testing, the epoch number is set to be 100 and some basic information of the model is shown in Table 1 below.



Figure 5 shows the loss function in training and validation sets, it can be seen that the loss is getting smaller and smaller as the training progresses. From Figure 5, in the late stage of model training, the distance between training loss curve and validation loss curve is really close and validation loss curve has no growth trend. These evidence shows that the underfitting and overfitting problems does not occur in this model and can be used for unseen data as well.

Table 1 Basic information of the model

Layer	Number of nodes	Activation function used
Input Layer	37	-
Hidden Layers	64	ReLU
	32	ReLU
	16	ReLU
Output layer	1	ReLU

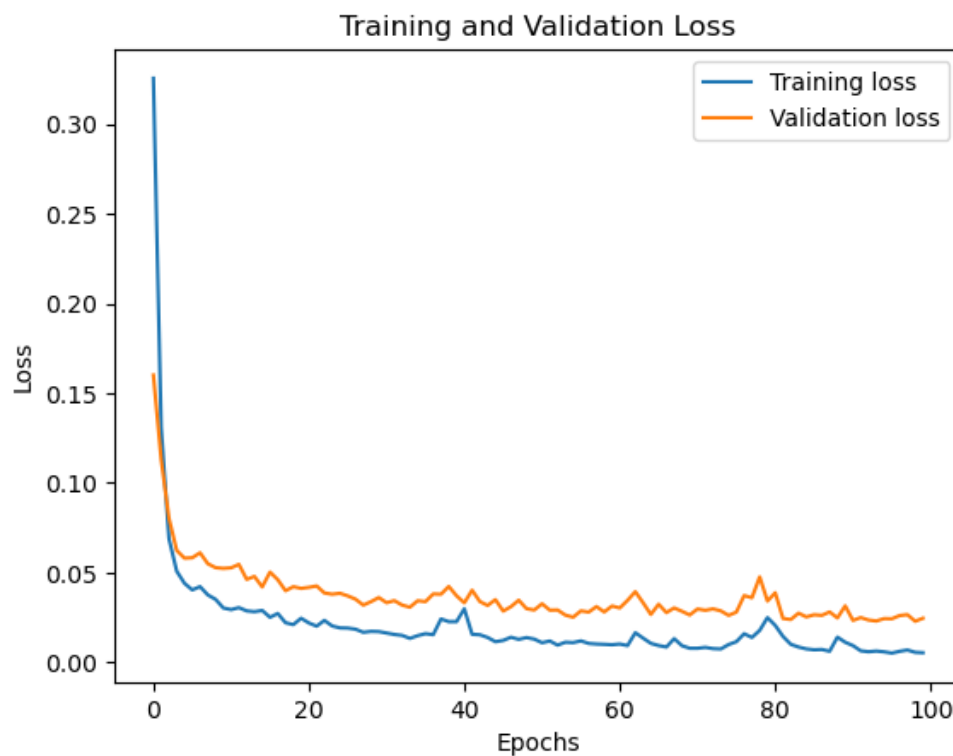


Figure 5 'Training and Validation loss' diagram of ANN model



There are 101 data used to test the performance of the model, and at the same time there are 101 wet packing density model prediction values to compare with the test values. The accuracy of predicted value can be calculated by using equation 1 below:

$$\text{Accuracy} = 1 - \left| \frac{\text{Predicted Value} - \text{Test Value}}{\text{Test Value}} \right| \quad (1)$$

The higher the accuracy value, the closer the value predicted by the model is to the actual value. For example, the true value of one of the 101 data sets is 0.8, and the value predicted by the model is 0.82123256. According to formula 1, the accuracy of this data set is 97.35%. The accuracy of the remaining 100 sets of data was calculated using the same equation. A complete table containing all the data accuracy is shown in Appendix D.

The final results can be divided into four categories. The accuracy of the first category of results is between 90% and 100%, and 67 of the 101 data sets are within this range. These 67 sets of data represent predicted values that are very close to the correct test values, which means that nearly two-thirds of the predictions are very accurate. These 67 sets of data show that the model has successfully learned the nonlinear relationship between various variables and wet packing density and can also give reliable predictions when faced with unseen data.

The accuracy of the second category is between 70% and 90% but not including 90%, and 20 of the 101 sets of data are within this range. These 20 sets of data predicted the values relatively accurately. Although the prediction effect of the second category of data is not as good as that of the first category, the accuracy of more than 70% is still within a relatively acceptable range, which means that the second category of data is still meaningful. These twenty sets of data show that the model has successfully learned most of the nonlinear relationships between various variables and wet packing density and can also give relatively reliable predictions when faced with new data.

The accuracy of the third category of data is less than but not equal to 70%, and 6 sets of data are within this range. The six data predicted by the model are significantly different from the real data, which means that the model has not successfully learned the relationship between different variables and wet packing density on these six sets of data. The main reason for this problem is that in order to avoid underfitting and overfitting problems, the data is split into three parts. The data used to train the model only accounts for 60% of the total



data, and this 60% of the data is randomly selected. The original data set contains experiments conducted by different researchers, and the variables affecting wet packing density recorded by each researcher are different, which results in only a small amount of data or even no data at all from the experiment conducted by a certain researcher being used to train the model. In other words, there will be insufficient data to train the model, and the model has not successfully learned the relationship between different variables and wet packing density in a series of data recorded by the experimenter. However, a large amount of data recorded by that researcher may be selected in the 20% test data, which will cause the wet packing density value recorded by that researcher to be unable to be accurately predicted.

The fourth category of data, which is the last category, is called 'abnormal data', and its accuracy cannot be obtained by equation 1. For example, the 25th and 33rd sets of data in Table 3 belong to this category. The true wet packing density value in the test data is 0, and when the true data is zero, equation 1 cannot give a result because the denominator is zero. Eight groups of data out of 101 test data are classified as the fourth category. This category of data appears because some researchers only recorded the values of different variables that determine wet packing density in the original data set, but the final wet packing density value was not displayed by the researchers. In the methodology section, it is mentioned that all blank data were replaced with 0 to train the model, so the values of all blank wet packing density became zero. As a result, some of the data with wet packing density of zero are also included in the randomly selected 60% training data and 20% test data. This also explains why there are data with test value of zero in Table 3. All data that cannot be calculated for accuracy due to a test value of 0 are marked as 'not applicable' in the accuracy section and are highlighted in yellow, as shown in Table 3. In addition, when the test value is zero, the corresponding data set is also highlighted as 'abnormal data'. Although the predicted value is also zero, the wet packing density value of zero is not in a reasonable range. However, since the model still successfully predicts the value of 0, its accuracy is retained.



Although not all the predicted values of the model are very accurate, but after calculation, the overall average prediction accuracy reaches 90.07%. This shows that for most data, the model can effectively fit the value of wet packing density. Overall, the ANN model trained in this project performs well on the training data, but the performance in the test data is somewhat reduced. In particular, the errors in individual sets of data are large, and the prediction results are not stable enough. It is preliminarily judged that these abnormal data have affected the prediction accuracy of the model. After the above analysis and classification, the performance of these 101 sets of data is summarised in Table 2.

Table 2 Accuracy of 101 sets of true value and predicted value of the model

	Accuracy (A)	Number of data	Proportion
Category 1	$90\% \leq A \leq 100\%$	67	66%
Category 2	$70\% \leq A < 90\%$	20	20%
Category 3	$< 70\%$	6	6%
Category 4 (abnormal data)	Not applicable	8	8%
Notes: Overall accuracy = 90.07%			

Table 3 Comparison of 41 sets of true value and predicted value of the model

No.	Test Value	Predicted Value	Accuracy	Category
1	0.8	0.82123256	97.35%	Category 1
2	0.8152	0.7789554	95.55%	Category 1
3	0.8258	0.89535743	91.58%	Category 1
4	0.8286	0.797423	96.24%	Category 1
5	0.80033267	0.8357218	95.58%	Category 1
6	0.8037	0.9171131	85.89%	Category 2
7	0.84318787	0.8298419	98.42%	Category 1
8	0	0	100.00%	Category 1 (Abnormal data)
9	0.8122	0.8545713	94.78%	Category 1
10	0.7999	0.85664207	92.91%	Category 1
11	0.8149753	0.65075266	79.85%	Category 2
12	0	0	100.00%	Category 1 (Abnormal data)
13	0.7958	0.82242745	96.65%	Category 1



14	0.8199	0.90162945	90.03%	Category 1
15	0.8132	0.9347548	85.05%	Category 2
16	0.7984	0.83404446	95.54%	Category 1
17	0.8234	0.8749365	93.74%	Category 1
18	0	0	100.00%	Category 1 (Abnormal data)
19	0.81	1.053328	69.96%	Category 3
20	0.8205	0.83784074	97.89%	Category 1
21	0.8177	0.02923717	3.58%	Category 3
22	0.83937	0.8898863	93.98%	Category 1
23	0.8189	0.9156254	88.19%	Category 2
24	0.8301	0.8732707	94.80%	Category 1
25	0	0.15230638	Not applicable	Abnormal Data
26	0.7995	0.8258638	96.70%	Category 1
27	0.80055976	0.1635645	20.43%	Category 3
28	0.8211	0.6922517	84.31%	Category 2
29	0.8047	0.69319236	86.14%	Category 2
30	0.8157857	0.731793	89.70%	Category 2
31	0.8393	0.8367627	99.70%	Category 1
32	0.8301	0.87722856	94.32%	Category 1
33	0	0.01497031	Not applicable	Abnormal Data
34	0.8144	0.96692204	81.27%	Category 2
35	0.8083	0.8394631	96.14%	Category 1
36	0.7926	0.8578852	91.76%	Category 1
37	0.8055	0.8394849	95.78%	Category 1
38	0.7937	0.8073123	98.28%	Category 1
39	0	0	100.00%	Category 1 (Abnormal data)
40	0	0	100.00%	Category 1 (Abnormal data)
41	0.8053	0.724901	90.02%	Category 1

A comparison of the 101 sets of true and predicted values for the complete model is shown in Appendix D.

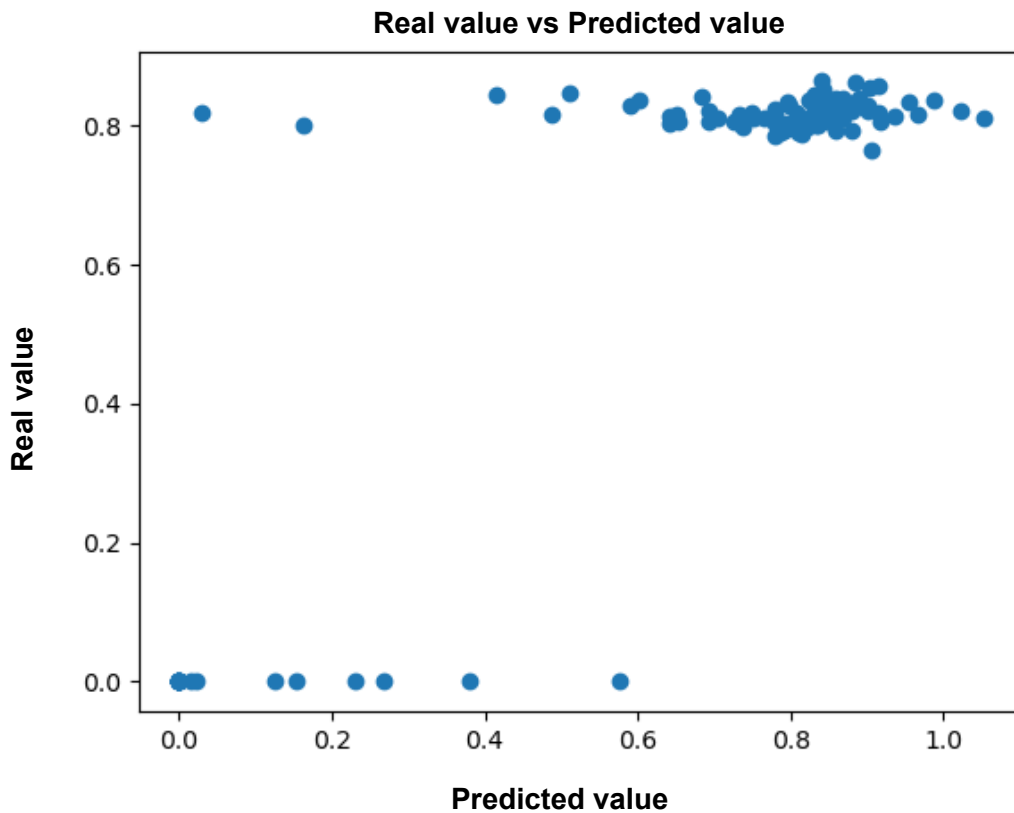


Figure 6 Scatterplot of real value vs predicted value of the model

To further examine the model's predictive performance, the scatter plot of the real data and predicted data is used to illustrate the performance of the model, as shown in Figure 6. The horizontal axis represents the predicted value of wet packing density given by the model, and the vertical axis represents the corresponding actual value. From the distribution of points in the scatter plot, most of the data points are concentrated in the upper right corner. In the original data set, almost all wet packing density values are between 0.75 and 0.86. At the same time, most of the predicted values are also around 0.8. The above information can be seen from the figure. Therefore, most of the data predicted by the model are reasonable. This further proves that the model has successfully learned most of the nonlinear connections between different variables and wet packing density and gives very accurate prediction results.

However, there are still a considerable number of points in the upper left corner, lower left corner and bottom middle area of Figure 6, and all the points in these sections are directly



caused by the emergence of abnormal data. Because the value of wet packing density is zero, there is no physical meaning. Therefore, all the points at the bottom of the scatter plot, that is, the test data, where the wet packing density is zero, are unreasonable. The data in the upper left corner of the scatter plot reveals that the actual wet packing density is around 0.8, but the result predicted by the model is less than 0.4, which is 50% lower. The interference of these abnormal data causes the model to over-learn these incorrect mapping relationships, resulting in misprediction of some data.

The values of coefficient of determination (R^2), Mean Absolute Error (MAE), Mean Square Error (MSE), and Root Mean Square Error (RMSE) of the scatter plot in Figure 6 were used to further evaluate the performance of the model. The following results are computed by Python code in Appendix C:

- $R^2 = 0.72932 \approx 73\%$
- $MAE = 0.09228 \approx 9.2\%$
- $MSE = 0.02650 = 2.65\%$
- $RMSE = 0.16278 \approx 16.3\%$

In this model, the value of R^2 is 0.72932 in the scatter plot, which shows that the ANN model can explain nearly 73% of the variance. This result shows that the prediction results of the model for most samples are close to the real data, which indicates the prediction of wet packing density and the true experimental result is moderately strongly correlated.

From the R^2 result, it can be seen that this ANN model has a strong fitting ability, but in this research project, the MAE value reached 9.2%. In the existing Kwan's model, the average MAE is only 2.2% (Du, Li, Pei, & Ma, 2021). This comparison shows that at the individual data level, the prediction error of the ANN model is greater than the Kwan's model. It is worth mentioning that this does not mean that this ANN model failed to give a relatively reasonable prediction, because the number of independent variables considered in Kwan's model is far less than the number of independent variables considered in the ANN model in this research. For example, Kwan's model does not take into account the impact of water and chemical on wet packing density, while the impact of water and chemical is included in this research project (Wong & Kwan, 2014) (Du, Li, Pei, & Ma, 2021). Since this model needs to learn more



nonlinear relationships between different independent variables and the dependent variable, which is the wet packing density, this situation potentially causes the prediction accuracy of the ANN model to decrease.

MSE refers to the average square error between the predicted value and the true value. This index can be used to measure the predictive performance of the model (N, 2025). The value of MSE is 2.65% in ANN model, which means the squared deviation between the predicted value given by the ANN model and the true value is 2.65%.

The RMSE is the squared error of the MSE, expressed as a mathematical equation is $RMSE = \sqrt{MSE}$ (Bobbitt, 2021). This index can more intuitively show the prediction accuracy of the model. The RMSE value of this model is 16.3%, which means that there is a 16.3% deviation between the ANN model and the true value. Although the MSE and RMSE values are not mentioned in Kwan's model, the MSE and RMSE of this ANN model can help future researchers compare the ANN model used in this study when training other models, so as to find a more optimised machine learning model.

By analysing the test data, prediction results and its accuracy, it can be found that there are some abnormal wet packing density data in the original data set. These wet packing density values are 0, which is much lower than most of the other wet packing density values. The reason for the appearance of 0 is that all blank data in the original data are replaced by 0 to accommodate the training of the ANN model. However, the appearance of zero wet packing density value greatly affects the training performance of the model. Especially because the ANN model needs to solve a regression problem, which is predicting the wet packing density, the Mean Square Error (MSE) is used as the loss function in the ANN model. The existence of abnormal data makes the model more sensitive to data with large errors, which causes the model to learn too much unnecessary connections between different variables and incorrect wet packing density values in the abnormal data (Yathish, 2022). This leads to a large deviation between the model's prediction of some predicted result and the real value. In other words, the root cause of model prediction errors is not entirely due to insufficient model capabilities or lack of training, but rather the presence of unreasonable abnormal data in the training data, that is, data with a wet packing density value of 0.



4.2 Limitations of the trained model and future investigation suggestion

Although the overall prediction result of the ANN model is satisfactory, and there are no underfitting and overfitting problems during the training process. However, some prediction results also show that this ANN model has certain limitations. One of the most important issues is that some of the predicted results are abnormally low, approaching or even equal to 0. However, a wet packing density of 0 has no actual physical meaning. As analysed in Section 4.1, the most prominent problem is the abnormal data in the training data and test data. Combined with the analysis of the preprocessing process in the methodology section above, it is found that the abnormal results appear because there are many missing wet packing density values in the original data, and these missing data are replaced by 0. The corresponding independent variable data that affects these wet packing densities filled with 0 are not missing. This directly leads to the fact that although these data contain the values of all the different independent variables recorded by the researcher in their experiment, it gives an unreasonable data of wet packing density of 0. The model over-learns these incorrect mapping relationships during the training process, which misleads the learning process and affects the prediction accuracy of the model. To further improve the performance of ANN models, the following are suggested three possible research directions:

1. If missing data is found, exclude it from the data in a timely manner in the pre-analysis stage to eliminate the misleading effect of abnormal data on model learning and thus affect the final prediction performance.
2. The number of training data used in this project is 301 sets, which is relatively small for the neural network model. In the future, more experimental data can be recorded and collected so that more data can be used to train the model and check the prediction performance of the model. More data can enable the ANN model to learn more detailed nonlinear relationships between various independent variables and wet packing density. Thereby improving the prediction accuracy of the ANN model.
3. In the future, try to use the random forest model to predict the value of wet packing density and compare it with the artificial neural network model used in this research. As mentioned in the literature review section above, the neural network was selected as the machine learning model for this study. The reason is that the random forest



model is more time-consuming and computationally expensive. However, these shortcomings of the random forest model do not necessarily affect its ability to predict wet packing density. Using the random forest model can verify whether it has more accurate and stable prediction performance under the same data conditions.

Therefore, the ANN model trained in this research has great potential. However, the appearance of some abnormal data affects its prediction accuracy. In the future, if more detailed research and improvement are carried out around the above three points, the ANN model or other machine learning models such as Random Forest model are expected to give higher accuracy and better performance.

5. Conclusion

This research trained an ANN model to predict the value of wet packing density, with the aim of exploring the accuracy and feasibility of the machine learning approach in predicting wet packing density. The performance of the model was evaluated by analysing the accuracy, scatter plots between real data and predicted data, R^2 , MAE, MSE and RMSE. The results show that the R^2 value on the test data is 73%, MAE is 9.2%, MSE is 2.65%, and RMSE is 16.3%, which means that the overall prediction results of the ANN model are relatively accurate. However, some prediction results of the model are abnormally low, even close to or equal to zero. After analysis, it was found that these unreasonable prediction results are caused by the fact that there are many missing values of wet packing density in the original data. During the training process, these missing values are replaced with zero and used for model training, which causes the ANN model to over-learn these incorrect mapping relationships during the training process. This directly leads to a decrease in the accuracy of the model's prediction results.

In summary, the ANN model trained in this research can accurately predict the value of wet packing density, and this model has great potential for improvement. Subsequent research can focus on clearing abnormal data in time before training the model, recording and collecting more data for training and testing the model, and trying to use the Random Forest model to build a new machine learning model using the same dataset to verify or compare



the model performance of the ANN model used in this research. Then the machine learning model can further improve the accuracy of predicting wet packing density.



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Appendix A: Full tables of series 1,2 and 3

Appendix A.1 Full table of series 1

Test number	Cementitious materials	SP added	Minimum voids ratio	Packing density
A1	OPC	No SP	0.831	0.546
A2		SP1	0.607	0.622
A3		SP2	0.705	0.586
A4	PFA	No SP	0.748	0.572
A5		SP1	0.547	0.646
A6		SP2	0.663	0.601
A7	CSF	No SP	0.916	0.522
A8		SP1	1.519	0.397
A9		SP2	0.843	0.543

(Wong & Kwan, Packing density of cementitious materials: part 2—packing and flow of OPC + PFA + CSF, 2007)

Appendix A.2 Full table of series 2

Test number	Cementitious materials (% by volume)			Minimum voids ratio	Packing density
	OPC	PFA	CSF		
B1	85	15	–	0.570	0.637
B2	70	30	–	0.560	0.641
B3	55	45	–	0.553	0.644
B4	40	60	–	0.556	0.643
B5	25	75	–	0.551	0.645
B6	85	–	15	0.422	0.703
B7	70	–	30	0.377	0.726
B8	55	–	45	0.490	0.671
B9	40	–	60	0.551	0.645
B10	25	–	75	0.696	0.590
B11	–	85	15	0.336	0.748
B12	–	70	30	0.342	0.745
B13	–	55	45	0.452	0.689
B14	–	40	60	0.740	0.575
B15	–	25	75	1.441	0.410

Note: SP1 added to all mixes



(Wong & Kwan, Packing density of cementitious materials: part 2—packing and flow of OPC + PFA + CSF, 2007)

Appendix A.3 Full table of series 3

Test number	Cementitious materials (% by volume)			Minimum voids ratio	Packing density
	OPC	PFA	CSF		
C1	70	15	15	0.392	0.718
C2	55	30	15	0.368	0.731
C3	40	45	15	0.370	0.730
C4	25	60	15	0.348	0.742
C5	55	15	30	0.358	0.736
C6	40	30	30	0.361	0.735
C7	25	45	30	0.330	0.752
C8	40	15	45	0.503	0.665
C9	25	30	45	0.447	0.691
C10	25	15	60	0.566	0.639

Note: SP1 added to all mixes

(Wong & Kwan, Packing density of cementitious materials: part 2—packing and flow of OPC + PFA + CSF, 2007)

Appendix B: Full dataset

No.	Specimens	SSCA content	SSFA content	RS content	IS content	QS content	FA content	SF content	GBFS content	WCP content	WGS content	RA	RFA	CaO content	MgO content	W/C M	Water	Cement	Fly ash	Silica fume	GBFS	WGP	WGS	RA	RFA	Natural sand	Iron sand	Granite (<10mm)	Granite (10-20mm)	SSCA (5-20mm)	SSFA (<5mm)	Q5	CaO	MgO	SP (%)	SP(kg)	Dosage/10 ³	Packing density	Void ratio	
	钟凌鹏	铜渣石比例	铜渣砂比例	河砂比例	铁砂比例	石灰砂比例	粉煤灰比例	硅粉比例	粒化高炉矿渣比例	玻璃粉比例	玻璃砂比例	再生粗骨料比例	再生细骨料比例						粉煤灰	硅粉	粒化高炉矿渣	玻璃粉	玻璃砂	再生粗骨料	再生细骨料	河砂	铁砂	小石	大石	铜渣石	铜渣砂	石英砂								
1	L						0%	0%	0%							0.60	260.1	433.6									795.0		405.0	405.0						0.05%	0.20	3.72	0.7736	0.2926
2	LSF5						0%	5%	0%							0.60	260.1	411.9		16.1							795.0		405.0	405.0						0.15%	0.64	7.95	0.8219	0.2181
3	LSF10						0%	10%	0%							0.60	260.1	390.2		32.2							795.0		405.0	405.0						0.21%	0.87	7.95	0.8361	0.1961
4	LSF15						0%	15%	0%							0.60	260.1	368.5		48.3							795.0		405.0	405.0						0.27%	1.10	8.05	0.8393	0.1915
5	LFA15						0%	0%	15%							0.60	260.1	368.5			60.4						795.0		405.0	405.0						0.05%	0.23	3.65	0.7973	0.2543
6	LFA25						0%	0%	25%							0.60	260.1	325.2			100.7						795.0		405.0	405.0						0.05%	0.22	3.56	0.7967	0.2552
7	LFA35						0%	0%	35%							0.60	260.1	281.8			141.0						795.0		405.0	405.0						0.05%	0.21	3.46	0.7990	0.2515
8	LGBFS15						15%	0%	0%							0.60	260.1	368.5		50.8							795.0		405.0	405.0						0.05%	0.23	4.71	0.2572	0.3513
9	LGBFS25						25%	0%	0%							0.60	260.1	325.2		84.6							795.0		405.0	405.0						0.06%	0.23	4.04	0.2509	0.3511
10	LGBFS35						35%	0%	0%							0.60	260.1	281.8		118.5							795.0		405.0	405.0						0.06%	0.23	4.17	0.2414	0.3509
11	LA						0%	0%	0%							0.60	260.1	433.6									795.0		405.0	405.0						0.02%	0.08	1.50	0.7960	0.2563
12	LSF3A						0%	5%	0%							0.60	260.1	411.9		16.1							795.0		405.0	405.0						0.03%	0.12	1.50	0.7965	0.2555
13	LSF10A						0%	10%	0%							0.60	260.1	390.2		32.2							795.0		405.0	405.0						0.04%	0.17	1.50	0.8003	0.2495
14	LSF15A						0%	15%	0%							0.60	260.1	368.5		48.3							795.0		405.0	405.0						0.05%	0.21	1.50	0.8019	0.2470
15	LGBFS15A						0%	0%	15%							0.60	260.1	368.5			60.4						795.0		405.0	405.0						0.02%	0.08	1.50	0.8011	0.2483
16	LGBFS25A						0%	0%	25%							0.60	260.1	325.2			100.7						795.0		405.0	405.0						0.02%	0.07	1.50	0.8011	0.2482
17	LGBFS35A						0%	0%	35%							0.60	260.1	281.8			141.0						795.0		405.0	405.0						0.02%	0.07	1.50	0.8044	0.2432
18	LFA15A						15%	0%	0%							0.60	260.1	368.5		50.8							795.0		405.0	405.0						0.02%	0.08	1.50	0.8043	0.2434
19	LFA25A						25%	0%	0%							0.60	260.1	325.2		84.6							795.0		405.0	405.0						0.02%	0.08	1.50	0.8089	0.2362
20	LFA35A						35%	0%	0%							0.60	260.1	281.8		118.5							795.0		405.0	405.0						0.02%	0.08	1.50	0.8139	0.2286
21	M						0%	0%	0%							0.40	221.4	553.6									795.0		405.0	405.0						0.14%	0.78	11.36	0.8055	0.2414
22	MSF5						0%	5%	0%							0.40	221.4	525.9		20.5							795.0		405.0	405.0						0.19%	1.04	12.00	0.8237	0.2140
23	MSF10						0%	10%	0%							0.40	221.4	498.2		41.1							795.0		405.0	405.0						0.32%	1.73	12.15	0.8293	0.2059
24	MSF15						0%	15%	0%							0.40	221.4	470.6		61.6							795.0		405.0	405.0						0.41%	2.16	12.06	0.8316	0.2025
25	MGBFS15						0%	0%	15%							0.40	221.4	470.6			77.1						795.0		405.0	405.0						0.14%	0.77	11.78	0.8085	0.2368
26	MGBFS25						0%	0%	25%							0.40	221.4	415.2			128.6						795.0		405.0	405.0						0.14%	0.77	12.19	0.8211	0.2179
27	MGBFS35						0%	0%	35%							0.40	221.4	359.8			180.0						795.0		405.0	405.0						0.14%	0.77	12.62	0.8151	0.2260
28	MFA15						15%	0%	0%							0.40	221.4	470.6		64.8							795.0		405.0	405.0						0.14%	0.76	11.02	0.8114	0.2324
29	MFA25						25%	0%	0%							0.40	221.4	415.2		108.0							795.0		405.0	405.0						0.14%	0.75	10.85	0.8166	0.2246
30	MFA35						35%	0%	0%							0.40	221.4	359.8		151.3							795.0		405.0	405.0						0.14%	0.74	10.67	0.8175	0.2233

备注: m1-筛底质量; m2-筛子总质量; m3-筛子+混凝土质量; m4-筛底+浆体质量。

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Zhengyi Zhang

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Machine Learning Approaches to Simulate and Predict Packing Density

Zhengyi Zhang

CIVL4600

伍凱捷

1	ISO-C100-0.11			100%	0%	0%	0%												795.0	405.0	405.0						0.11%	0.61		0.7891	0.2673
2	ISO-C100-0.22			100%	0%	0%	0%												795.0	405.0	405.0						0.22%	1.22		0.7900	0.2658
3	ISO-C100-0.31			100%	0%	0%	0%												795.0	405.0	405.0						0.31%	1.72		0.8047	0.2427
4	ISO-C100-0.42			100%	0%	0%	0%												795.0	405.0	405.0						0.42%	2.33		0.7994	0.2509
5	ISO-C100-0.54			100%	0%	0%	0%												795.0	405.0	405.0						0.54%	2.99			
6	ISSO-C100-0.11			50%	50%	0%	0%												397.5	1067.6	405.0	405.0					0.11%	0.61		0.7928	0.2614
7	ISSO-C100-0.22			50%	50%	0%	0%												397.5	1067.6	405.0	405.0					0.22%	1.22		0.7982	0.2528
8	ISSO-C100-0.31			50%	50%	0%	0%												397.5	1067.6	405.0	405.0					0.31%	1.72			
9	ISSO-C100-0.42			50%	50%	0%	0%												397.5	1067.6	405.0	405.0					0.42%	2.33			
10	ISSO-C100-0.54			50%	50%	0%	0%												397.5	1067.6	405.0	405.0					0.54%	2.99			
11	IS100-C100-0.11			0%	100%	0%	0%												0.0	2135.1	405.0	405.0					0.11%	0.61		0.8031	0.2452
12	IS100-C100-0.22			0%	100%	0%	0%												0.0	2135.1	405.0	405.0					0.22%	1.22		0.7960	0.2563
13	IS100-C100-0.31			0%	100%	0%	0%												0.0	2135.1	405.0	405.0					0.31%	1.72			
14	IS100-C100-0.42			0%	100%	0%	0%												0.0	2135.1	405.0	405.0					0.42%	2.33			
15	IS100-C100-0.54			0%	100%	0%	0%												0.0	2135.1	405.0	405.0					0.54%	2.99			
16	ISSO-SF3-0.11			50%	50%	0%	5%					20.5							397.5	1067.6	405.0	405.0					0.11%	0.60		0.7918	0.2629
17	ISSO-SF3-0.22			50%	50%	0%	5%					20.5							397.5	1067.6	405.0	405.0					0.22%	1.20		0.7837	0.2599
18	ISSO-SF3-0.31			50%	50%	0%	5%					20.5							397.5	1067.6	405.0	405.0					0.31%	1.69		0.7873	0.2542
19	ISSO-SF3-0.42			50%	50%	0%	5%					20.5							397.5	1067.6	405.0	405.0					0.42%	2.30		0.7904	0.2652
20	ISSO-SF3-0.54			50%	50%	0%	5%					20.5							397.5	1067.6	405.0	405.0					0.54%	2.95			
21	ISSO-SF10-0.11			50%	50%	0%	10%					41.1							397.5	1067.6	405.0	405.0					0.11%	0.59		0.7893	0.2669
22	ISSO-SF10-0.22			50%	50%	0%	10%					41.1							397.5	1067.6	405.0	405.0					0.22%	1.19		0.7908	0.2645
23	ISSO-SF10-0.31			50%	50%	0%	10%					41.1							397.5	1067.6	405.0	405.0					0.31%	1.67		0.8001	0.2498
24	ISSO-SF10-0.42			50%	50%	0%	10%					41.1							397.5	1067.6	405.0	405.0					0.42%	2.27		0.7930	0.2610
25	ISSO-SF10-0.54			50%	50%	0%	10%					41.1							397.5	1067.6	405.0	405.0					0.54%	2.91			
26	ISSO-SF15-0.11			50%	50%	0%	15%					61.6							397.5	1067.6	405.0	405.0					0.11%	0.59		0.7862	0.2719
27	ISSO-SF15-0.22			50%	50%	0%	15%					61.6							397.5	1067.6	405.0	405.0					0.22%	1.17		0.7873	0.2702
28	ISSO-SF15-0.31			50%	50%	0%	15%					61.6							397.5	1067.6	405.0	405.0					0.31%	1.65		0.7925	0.2618
29	ISSO-SF15-0.42			50%	50%	0%	15%					61.6							397.5	1067.6	405.0	405.0					0.42%	2.24		0.8006	0.2491
30	ISSO-SF15-0.54			50%	50%	0%	15%					61.6							397.5	1067.6	405.0	405.0					0.54%	2.87		0.8064	0.2401
31	IS100-SF5-0.11			0%	100%	0%	5%					20.5							0.0	2135.1	405.0	405.0					0.11%	0.60		0.7992	0.2513
32	IS100-SF5-0.22			0%	100%	0%	5%					20.5							0.0	2135.1	405.0	405.0					0.22%	1.20		0.8017	0.2473
33	IS100-SF5-0.31			0%	100%	0%	5%					20.5							0.0	2135.1	405.0	405.0					0.31%	1.69		0.8007	0.2489
34	IS100-SF5-0.42			0%	100%	0%	5%					20.5							0.0	2135.1	405.0	405.0					0.42%	2.30		0.7981	0.2530
35	IS100-SF5-0.54			0%	100%	0%	5%					20.5							0.0	2135.1	405.0	405.0					0.54%	2.95			
36	IS100-SF10-0.11			0%	100%	0%	10%					41.1							0.0	2135.1	405.0	405.0					0.11%	0.59		0.7948	0.2582
37	IS100-SF10-0.22			0%	100%	0%	10%					41.1							0.0	2135.1	405.0	405.0					0.22%	1.19		0.8005	0.2492
38	IS100-SF10-0.31			0%	100%	0%	10%					41.1							0.0	2135.1	405.0	405.0					0.31%	1.67		0.8114	0.2324
39	IS100-SF10-0.42			0%	100%	0%	10%					41.1							0.0	2135.1	405.0	405.0					0.42%	2.27		0.8000	0.2500
40	IS100-SF10-0.54			0%	100%	0%	10%					41.1							0.0	2135.1	405.0	405.0					0.54%	2.91			
41	IS100-SF15-0.11			0%	100%	0%	15%					61.6							0.0	2135.1	405.0	405.0					0.11%	0.59		0.7911	0.2641
42	IS100-SF15-0.22			0%	100%	0%	15%					61.6							0.0	2135.1	405.0	405.0					0.22%	1.17		0.7926	0.2617
43	IS100-SF15-0.31			0%	100%	0%	15%					61.6							0.0	2135.1	405.0	405.0					0.31%	1.65		0.8089	0.2362



Machine Learning Approaches to Simulate and Predict Packing Density

Zhengyi Zhang

CIVL4600

44	IS100-SF15-0.42			0%	100%		0%	15%								0.40	221.4	470.6		61.6									0.0	2135.1	405.0	405.0							0.42%	2.24		0.8013	0.2480		
45	IS100-SF15-0.54			0%	100%		0%	15%								0.40	221.4	470.6		61.6										0.0	2135.1	405.0	405.0							0.54%	2.87		0.8002	0.2497	
46	IS50-FA15-0.11			50%	50%		15%	0%								0.40	221.4	470.6	64.8											397.5	1067.6	405.0	405.0							0.11%	0.59		0.7826	0.2778	
47	IS50-FA15-0.22			50%	50%		15%	0%								0.40	221.4	470.6	64.8											397.5	1067.6	405.0	405.0							0.22%	1.18		0.7976	0.2538	
48	IS50-FA15-0.31			50%	50%		15%	0%								0.40	221.4	470.6	64.8											397.5	1067.6	405.0	405.0							0.31%	1.66				
49	IS50-FA15-0.42			50%	50%		15%	0%								0.40	221.4	470.6	64.8											397.5	1067.6	405.0	405.0							0.42%	2.25				
50	IS50-FA15-0.54			50%	50%		15%	0%								0.40	221.4	470.6	64.8											397.5	1067.6	405.0	405.0							0.54%	2.89				
51	IS50-FA25-0.11			50%	50%		25%	0%								0.40	221.4	415.2	108.0											397.5	1067.6	405.0	405.0							0.11%	0.58		0.7790	0.2837	
52	IS50-FA25-0.22			50%	50%		25%	0%								0.40	221.4	415.2	108.0											397.5	1067.6	405.0	405.0							0.22%	1.15		0.7968	0.2550	
53	IS50-FA25-0.31			50%	50%		25%	0%								0.40	221.4	415.2	108.0											397.5	1067.6	405.0	405.0							0.31%	1.62				
54	IS50-FA25-0.42			50%	50%		25%	0%								0.40	221.4	415.2	108.0											397.5	1067.6	405.0	405.0							0.42%	2.20				
55	IS50-FA25-0.54			50%	50%		25%	0%								0.40	221.4	415.2	108.0											397.5	1067.6	405.0	405.0							0.54%	2.83				
56	IS50-FA35-0.11			50%	50%		35%	0%								0.40	221.4	359.8	151.3											397.5	1067.6	405.0	405.0							0.11%	0.56		0.7631	0.3104	
57	IS50-FA35-0.22			50%	50%		35%	0%								0.40	221.4	359.8	151.3											397.5	1067.6	405.0	405.0							0.22%	1.12		0.7731	0.2935	
58	IS50-FA35-0.31			50%	50%		35%	0%								0.40	221.4	359.8	151.3											397.5	1067.6	405.0	405.0							0.31%	1.58		0.7572	0.3207	
59	IS50-FA35-0.42			50%	50%		35%	0%								0.40	221.4	359.8	151.3											397.5	1067.6	405.0	405.0							0.42%	2.15				
60	IS50-FA35-0.54			50%	50%		35%	0%								0.40	221.4	359.8	151.3											397.5	1067.6	405.0	405.0							0.54%	2.76				
61	IS100-FA15-0.11			0%	100%		15%	0%								0.40	221.4	470.6	64.8											0.0	2135.1	405.0	405.0							0.11%	0.59		0.7881	0.2689	
62	IS100-FA15-0.22			0%	100%		15%	0%								0.40	221.4	470.6	64.8											0.0	2135.1	405.0	405.0							0.22%	1.18				
63	IS100-FA15-0.31			0%	100%		15%	0%								0.40	221.4	470.6	64.8											0.0	2135.1	405.0	405.0							0.31%	1.66				
64	IS100-FA15-0.42			0%	100%		15%	0%								0.40	221.4	470.6	64.8											0.0	2135.1	405.0	405.0							0.42%	2.25				
65	IS100-FA15-0.54			0%	100%		15%	0%								0.40	221.4	470.6	64.8											0.0	2135.1	405.0	405.0							0.54%	2.89				
66	IS100-FA25-0.11			0%	100%		25%	0%								0.40	221.4	415.2	108.0											0.0	2135.1	405.0	405.0							0.11%	0.58		0.7865	0.2715	
67	IS100-FA25-0.22			0%	100%		25%	0%								0.40	221.4	415.2	108.0											0.0	2135.1	405.0	405.0							0.22%	1.15				
68	IS100-FA25-0.31			0%	100%		25%	0%								0.40	221.4	415.2	108.0											0.0	2135.1	405.0	405.0							0.31%	1.62				
69	IS100-FA25-0.42			0%	100%		25%	0%								0.40	221.4	415.2	108.0											0.0	2135.1	405.0	405.0							0.42%	2.20				
70	IS100-FA25-0.54			0%	100%		25%	0%								0.40	221.4	415.2	108.0											0.0	2135.1	405.0	405.0							0.54%	2.83				
71	IS100-FA35-0.11			0%	100%		35%	0%								0.40	221.4	359.8	151.3											0.0	2135.1	405.0	405.0							0.11%	0.56		0.7862	0.2719	
72	IS100-FA35-0.22			0%	100%		35%	0%								0.40	221.4	359.8	151.3											0.0	2135.1	405.0	405.0							0.22%	1.12		0.7851	0.2737	
73	IS100-FA35-0.31			0%	100%		35%	0%								0.40	221.4	359.8	151.3											0.0	2135.1	405.0	405.0							0.31%	1.58				
74	IS100-FA35-0.42			0%	100%		35%	0%								0.40	221.4	359.8	151.3											0.0	2135.1	405.0	405.0							0.42%	2.15				
75	IS100-FA35-0.54			0%	100%		35%	0%								0.40	221.4	359.8	151.3											0.0	2135.1	405.0	405.0							0.54%	2.76				

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	GP35-GS0									35%	0%					0.4	221.4	359.8	—		150.0	—							795.0		405.0	405.0					0.20%				0.8441	0.1847
5	GP9-CS50									0%	50%					0.4	221.4	533.6	—			180.0									405.0	405.0							0.20%		0.8164	0.2249
6	GP15-GS50									15%	50%					0.4	221.4	470.6	—		64.3	180.0								397.5		405.0	405.0					0.20%		0.8308	0.2036	
7	GP25-GS50									25%	50%					0.4	221.4	415.2	—		107.2	180.0								397.5		405.0	405.0					0.20%		0.8409	0.1892	
8	GP35-GS50									35%	50%					0.4	221.4	359.8	—			150.0	180.0							397.5		405.0	405.0					0.20%		0.8444	0.1842	
9	GP9-CSI100									0%	100%					0.4	221.4	533.6	—		—	360.0								—		405.0	405.0					0.20%		0.8088	0.2365	
10	GP15-CSI100									15%	100%					0.4	221.4	470.6	—		64.3	360.0								—		405.0	405.0					0.20%		0.8106	0.2337	
11	GP25-CSI100									25%	100%					0.4	221.4	415.2	—			107.2	360.0							—		405.0	405.0					0.20%		0.8267	0.2097	
12	GP35-CSI100									35%	100%					0.4	221.4	359.8	—			150.0	360.0							—		405.0	405.0					0.20%		0.8286	0.2068	
13	GP35-CSI100-SF5									35%	100%					0.4	221.4	332.2	—		20.5	150.0	360.0							—		405.0	405.0					0.20%		0.8320	0.2020	
14	GP35-CSI100-SF10									35%	100%					0.4	221.4	304.5	—		41.1	150.0	360.0							—		405.0	405.0					0.20%		0.8391	0.1917	
15	GP35-CSI100-SF15									35%	100%					0.4	221.4	276.8	—		61.6	150.0	360.0							—		405.0	405.0					0.20%		0.8272	0.2089	
16	GP35-CSI100-SF20									35%	100%					0.4	221.4	249.1	—		82.2	150.0	360.0							—		405.0	405.0					0.20%		0.8217	0.2170	

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47	GP35-GS100-0.3			0%			0%		35%	100%				0.4	221.4	359.8	—		150.0	360.0			—		405.0	405.0					0.40%				
48	GP35-GS100-0.4			0%			0%		35%	100%				0.4	221.4	359.8	—		150.0	360.0			—		405.0	405.0					0.50%				
49	GP35-GS100-SF3-0.2			0%			5%		35%	100%				0.4	221.4	332.2	20.5		150.0	360.0			—		405.0	405.0					0.20%			0.8320	
50	GP35-GS100-SF3-0.3			0%			5%		35%	100%				0.4	221.4	332.2	20.5		150.0	360.0			—		405.0	405.0					0.30%			0.8426	
51	GP35-GS100-SF3-0.4			0%			5%		35%	100%				0.4	221.4	332.2	20.5		150.0	360.0			—		405.0	405.0					0.40%				
52	GP35-GS100-SF3-0.5			0%			5%		35%	100%				0.4	221.4	332.2	20.5		150.0	360.0			—		405.0	405.0					0.50%				
53	GP35-GS100-SF10-0.2			0%			10%		35%	100%				0.4	221.4	304.5	41.1		150.0	360.0			—		405.0	405.0					0.20%			0.8391	
54	GP35-GS100-SF10-0.3			0%			10%		35%	100%				0.4	221.4	304.5	41.1		150.0	360.0			—		405.0	405.0					0.30%			0.8493	
55	GP35-GS100-SF10-0.4			0%			10%		35%	100%				0.4	221.4	304.5	41.1		150.0	360.0			—		405.0	405.0					0.40%				
56	GP35-GS100-SF10-0.5			0%			10%		35%	100%				0.4	221.4	304.5	41.1		150.0	360.0			—		405.0	405.0					0.50%				
57	GP35-GS100-SF15-0.2			0%			15%		35%	100%				0.4	221.4	276.8	61.6		150.0	360.0			—		405.0	405.0					0.20%			0.8272	
58	GP35-GS100-SF15-0.3			0%			15%		35%	100%				0.4	221.4	276.8	61.6		150.0	360.0			—		405.0	405.0					0.30%			0.8388	
59	GP35-GS100-SF15-0.4			0%			15%		35%	100%				0.4	221.4	276.8	61.6		150.0	360.0			—		405.0	405.0					0.40%			0.8407	
60	GP35-GS100-SF15-0.5			0%			15%		35%	100%				0.4	221.4	276.8	61.6		150.0	360.0			—		405.0	405.0					0.50%			0.8424	
61	GP35-GS100-SF20-0.2			0%			20%		35%	100%				0.4	221.4	249.1	82.2		150.0	360.0			—		405.0	405.0					0.20%				
62	GP35-GS100-SF20-0.3			0%			20%		35%	100%				0.4	221.4	249.1	82.2		150.0	360.0			—		405.0	405.0					0.30%			0.8335	
63	GP35-GS100-SF20-0.4			0%			20%		35%	100%				0.4	221.4	249.1	82.2		150.0	360.0			—		405.0	405.0					0.40%			0.8357	
64	GP35-GS100-SF20-0.5			0%			20%		35%	100%				0.4	221.4	249.1	82.2		150.0	360.0			—		405.0	405.0					0.50%			0.8413	

陈宇升

1	NC0.6-0														0.60	260.1	433.6							0.0		795.0		405.0	405.0					0.05%			0.8364	0.1956
2	RAC0.6-25														0.60	260.1	433.6							189.4		795.0		303.8	303.8					0.05%			0.8339	0.1991
3	RAC0.6-50														0.60	260.1	433.6							378.8		795.0		202.5	202.5					0.05%			0.8278	0.2080
4	RAC0.6-75														0.60	260.1	433.6							568.1		795.0		101.3	101.3					0.05%			0.8258	0.2110
5	RAC0.6-100														0.60	260.1	433.6							757.5		795.0		0.0	0.0					0.05%			0.8213	0.2175
6	RAC0.6-100-SF5														0.60	260.1	411.9		16.1					757.5		795.0		0.0	0.0					0.05%			0.8234	0.2145
7	RAC0.6-100-SF10														0.60	260.1	390.2		32.2					757.5		795.0		0.0	0.0					0.05%			0.8271	0.2090
8	NC0.4-0														0.40	221.4	553.6							0.0		795.0		405.0	405.0					0.20%			0.8264	0.2100
9	RAC0.4-25														0.40	221.4	553.6							189.4		795.0		303.8	303.8					0.20%			0.8218	0.2168
10	RAC0.4-50														0.40	221.4	553.6							378.8		795.0		202.5	202.5					0.20%			0.8199	0.2196
11	RAC0.4-75														0.40	221.4	553.6							568.1		795.0		101.3	101.3					0.20%			0.8173	0.2235
12	RAC0.4-100														0.40	221.4	553.6							757.5		795.0		0.0	0.0					0.20%			0.8112	0.2327
13	RAC0.4-100-SF5														0.40	221.4	525.9		20.5					757.5		795.0		0.0	0.0					0.20%			0.8160	0.2255
14	RAC0.4-100-SF10														0.40	221.4	498.2		41.1					757.5		795.0		0.0	0.0					0.20%			0.8191	0.2209
15	NC0.2-0														0.20	153.1	765.4							0.0		795.0		405.0	405.0					2.50%			0.8600	0.1629
16	RAC0.2-25														0.20	153.1	765.4							189.4		795.0		303.8	303.8					2.50%			0.8567	0.1673
17	RAC0.2-50														0.20	153.1	765.4							378.8		795.0		202.5	202.5					2.50%			0.8536	0.1716
18	RAC0.2-75														0.20	153.1	765.4							568.1		795.0		101.3	101.3					2.50%			0.8503	0.1760
19	RAC0.2-100														0.20	153.1	765.4							757.5		795.0		0.0	0.0					2.50%			0.8462	0.1818

钟箭

1	0.4-NC														0.40	221.00	554.00										795.00		405.00	405.00						0.25%			0.8288	0.2066
2	0.6-NC														0.60	260.00	434.00										795.00		405.00	405.00						0.10%			0.8307	0.2038
3	0.4-SSCA25														0.40	221.00	554.00										795.00		304.00	304.00		253.00				0.25%			0.8351	0.1975
4	0.4-SSCA50														0.40	221.00	554.00										795.00		203.00	203.00		506.00				0.25%			0.8376	0.1940
5	0.4-SSCA75														0.40	221.00	554.00										795.00		101.00	101.00		758.00				0.25%			0.8340	0.1990
6	0.4-SSCA100														0.40	221.00	554.00										795.00		0.00	0.00		1011.00				0.25%			0.8335	0.1997
7	0.6-SSCA25														0.60	260.00	434.00										795.00		304.00	304.00		253.00				0.10%			0.8339	0.1993
8	0.6-SSCA50														0.60	260.00	434.00										795.00		203.00	203.00		506.00				0.10%			0.8356	0.1967
9	0.6-SSCA75														0.60	260.00	434.00										795.00		101.00	101.00		758.00				0.10%			0.8334	0.1999
10	0.6-SSCA100														0.60	260.00	434.00										795.00		0.00	0.00		1011.00				0.10%			0.8312	0.2031
11	0.4-SSCA100-SF5														0.40	221.00	526.00		21.00								795.00		0.00	0.00		1011.00				0.25%			0.8355	0.1968
12	0.4-SSCA100-SF10														0.40	221.00	498.00		41.00								795.00		0.00	0.00		1011.00				0.25%			0.8381	0.1931
13	0.4-SSCA100-SF15														0.40	221.00	471.00		62.00								795.00		0.00	0.00		1011.00				0.25%			0.8355	0.1969
14	0.6-SSCA100-SF5														0.60	260.00	412.00		16.00								795.00		0.00	0.00		1011.00				0.10%			0.8394	0.1914
15	0.6-SSCA100-SF10														0.60	260.00	390.00		32.00								795.00		0.00	0.00		1011.00				0.10%			0.8414	0.1884
16	0.6-SSCA100-SF15														0.60	260.00	269.00		48.00								795.00		0.00	0.00		1011.00				0.10%			0.8375	0.1940

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张伯熙

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谢煜明

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Appendix C: Python code used to train the model

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

from keras.models import Sequential
from keras.layers import Input, Dense, Dropout
from keras import optimizers
import sklearn
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.metrics import r2_score, mean_absolute_error, mean_squared_error

input_data = pd.read_excel('Mix_Design_WPD.xlsx',
                           skiprows=[1,2,33,34,35,66,67,68,79,80,81,100,101,102,103,133,134,153,154,155,201,202,203,
                                       279,280,281,304,305,322,323,324,389,390,391,411,412,413,430,431,432,448,449,450,
                                       463,464,465]
                           , usecols="A:AL,AT,AU",na_values=["-", "-"])
                           #"A:D,G:J,Q:V,AA,AC:AG,AJ:AU")
input_data.fillna(0, inplace=True)
#input_data.fillna('-', inplace=True)
data_group1 = input_data#.iloc[0:278]
display(data_group1)

y = data_group1['Packing\ndensity'].copy()
X = data_group1.copy()
X.drop(['No.', 'Specimens', 'Packing\ndensity'], axis=1, inplace=True)

X_train, X_test, y_train, y_test = train_test_split(X.values, y.values, test_size=0.2)
X_train, X_valid, y_train, y_valid = train_test_split(X_train, y_train, test_size=0.25)

#X = scaler.fit_transform(X)
#scaler1 = StandardScaler()
#y = data_group1['Packing\ndensity'].values
#y = scaler1.fit_transform(y.reshape(-1,1))

scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_valid = scaler.transform(X_valid)
X_test = scaler.transform(X_test)

model = Sequential()
model.add(Input(shape=(X_train.shape[1],)))
model.add(Dense(64, activation='relu'))
model.add(Dense(32, activation='relu'))
model.add(Dense(16, activation='relu'))
#model.add(Dense(8, activation='relu'))
model.add(Dense(1, activation='relu'))

model.compile(loss='mse', optimizer=optimizers.Adam(learning_rate=0.001))

X_train = X_train.astype(np.float32)
X_valid = X_valid.astype(np.float32)
X_test = X_test.astype(np.float32)
y_train = y_train.astype(np.float32)
y_valid = y_valid.astype(np.float32)
y_test = y_test.astype(np.float32)

history = model.fit(X_train, y_train, epochs=100, batch_size=20, validation_data=(X_valid, y_valid))
```



```
plt.plot(history.history['loss'], label='Training loss')
plt.plot(history.history['val_loss'], label='Validation loss')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.legend()
plt.title('Training and Validation Loss')
plt.show()
```

```
mse_test = model.evaluate(X_test, y_test)
print("mse: ", mse_test)
y_preid = model.predict(X_test)
plt.scatter(y_preid, y_test)
```

```
r2_ffn = r2_score(y_test, y_preid)
mae_ffn = mean_absolute_error(y_test, y_preid)
mse_ffn = mean_squared_error(y_test, y_preid)
rmse_ffn = np.sqrt(mse_ffn)

print("Metrics for the FFN model:")
print(f" R2_ffn: {r2_ffn}")
print(f" MAE_ffn: {mae_ffn}")
print(f" MSE_ffn: {mse_ffn}")
print(f" RMSE_ffn: {rmse_ffn}")
```

```
print(y_test)
```

```
print(y_preid)
```



Appendix D: Full table on test value, predicted value and accuracy

No.	Test Value	Predicted Value	Accuracy	Category
1	0.8	0.82123256	97.35%	Category 1
2	0.8152	0.7789554	95.55%	Category 1
3	0.8258	0.89535743	91.58%	Category 1
4	0.8286	0.797423	96.24%	Category 1
5	0.80033267	0.8357218	95.58%	Category 1
6	0.8037	0.9171131	85.89%	Category 2
7	0.84318787	0.8298419	98.42%	Category 1
8	0	0	100.00%	Category 1 (Abnormal data)
9	0.8122	0.8545713	94.78%	Category 1
10	0.7999	0.85664207	92.91%	Category 1
11	0.8149753	0.65075266	79.85%	Category 2
12	0	0	100.00%	Category 1 (Abnormal data)
13	0.7958	0.82242745	96.65%	Category 1
14	0.8199	0.90162945	90.03%	Category 1
15	0.8132	0.9347548	85.05%	Category 2
16	0.7984	0.83404446	95.54%	Category 1
17	0.8234	0.8749365	93.74%	Category 1
18	0	0	100.00%	Category 1 (Abnormal data)
19	0.81	1.053328	69.96%	Category 3
20	0.8205	0.83784074	97.89%	Category 1
21	0.8177	0.02923717	3.58%	Category 3
22	0.83937	0.8898863	93.98%	Category 1
23	0.8189	0.9156254	88.19%	Category 2
24	0.8301	0.8732707	94.80%	Category 1
25	0	0.15230638	Not applicable	Abnormal Data
26	0.7995	0.8258638	96.70%	Category 1
27	0.80055976	0.1635645	20.43%	Category 3
28	0.8211	0.6922517	84.31%	Category 2
29	0.8047	0.69319236	86.14%	Category 2
30	0.8157857	0.731793	89.70%	Category 2
31	0.8393	0.8367627	99.70%	Category 1
32	0.8301	0.87722856	94.32%	Category 1
33	0	0.01497031	Not applicable	Abnormal Data
34	0.8144	0.96692204	81.27%	Category 2
35	0.8083	0.8394631	96.14%	Category 1
36	0.7926	0.8578852	91.76%	Category 1
37	0.8055	0.8394849	95.78%	Category 1



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38	0.7937	0.8073123	98.28%	Category 1
39	0	0	100.00%	Category 1 (Abnormal data)
40	0	0	100.00%	Category 1 (Abnormal data)
41	0.8053	0.724901	90.02%	Category 1
42	0.8385	0.8691573	96.34%	Category 1
43	0.7976	0.7980671	99.94%	Category 1
44	0.8532	0.9020185	94.28%	Category 1
45	0	0	100.00%	Category 1 (Abnormal data)
46	0.8349	0.9862848	81.87%	Category 2
47	0.7893	0.7871972	99.73%	Category 1
48	0.7873	0.8132717	96.70%	Category 1
49	0	0.57650465	Not applicable	Abnormal Data
50	0.8108	0.86732346	93.03%	Category 1
51	0	0.26866227	Not applicable	Abnormal Data
52	0.8251	0.83074003	99.32%	Category 1
53	0.7904	0.8091397	97.63%	Category 1
54	0.8357	0.6019822	72.03%	Category 2
55	0.8284	0.85372263	96.94%	Category 1
56	0.8191	1.021272	75.32%	Category 2
57	0.809591	0.7646962	94.45%	Category 1
58	0.8172	0.80725354	98.78%	Category 1
59	0.8065	0.82216257	98.06%	Category 1
60	0	0.23004207	Not applicable	Abnormal Data
61	0.7631	0.9053249	81.36%	Category 2
62	0	0	100.00%	Category 1 (Abnormal data)
63	0.8601306	0.8854482	97.06%	Category 1
64	0.8029	0.77877194	96.99%	Category 1
65	0.8286	0.5907586	71.30%	Category 2
66	0	0.02229195	Not applicable	Abnormal Data
67	0.8273	0.9003385	91.17%	Category 1
68	0.8089	0.830432	97.34%	Category 1
69	0.8339	0.79515386	95.35%	Category 1
70	0.8567	0.9158511	93.10%	Category 1
71	0	0	100.00%	Category 1 (Abnormal data)
72	0.8042539	0.6525287	81.13%	Category 2
73	0	0.38035697	Not applicable	Abnormal Data
74	0	0	100.00%	Category 1
75	0.7976	0.73835874	92.57%	Category 1
76	0.8444	0.41539848	49.19%	Category 3
77	0.7851	0.7793609	99.27%	Category 1
78	0.8123	0.64087886	78.90%	Category 2



79	0.8395	0.68401176	81.48%	Category 2
80	0.8213	0.8795325	92.91%	Category 1
81	0.8224	0.78028876	94.88%	Category 1
82	0.8101	0.70398045	86.90%	Category 2
83	0.7918	0.79028505	99.81%	Category 1
84	0.83561	0.82392746	98.60%	Category 1
85	0.7911	0.8792055	88.86%	Category 2
86	0.85084057	0.84174156	98.93%	Category 1
87	0.8006	0.8006735	99.99%	Category 1
88	0.8626032	0.83935404	97.30%	Category 1
89	0.8167966	0.74912244	91.71%	Category 1
90	0.8148	0.85912544	94.56%	Category 1
91	0	0	100.00%	Category 1 (Abnormal data)
92	0.8089	0.81776625	98.90%	Category 1
93	0.8145	0.486685	59.75%	Category 3
94	0.8325	0.95545864	85.23%	Category 2
95	0.8026	0.64069176	79.83%	Category 2
96	0.8172	0.850122	95.97%	Category 1
97	0	0.12583	Not applicable	Abnormal Data
98	0.8448	0.5115041	60.55%	Category 3
99	0.83751	0.85794675	97.56%	Category 1
100	0.8092	0.75062394	92.76%	Category 1
101	0.8028	0.79366887	98.86%	Category 1