Machine-Learning-Aided Prediction of Flexural Strength and ASR Expansion for Waste Glass Cementitious Composite

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Abstract: Waste glass (WG) is unsustainable due to its nonbiodegradable property. However, its main ingredient is silicon dioxide, which can be utilised as a supplementary cementitious material. Before reusing WG, the flexural strength (FS) and alkali–silica reaction (ASR) expansion of WG concrete are two essential properties that must be investigated. This study produced mortar containing activated glass powder using mechanical, chemical, and mechanical–chemical (combined) approaches. The results showed that mortar containing 30% WG powder using the combined method was optimal for improving the FS and mitigating the ASR expansion. The microstructure analysis was implemented to explore the activation effect on the glass powder and mortar. Moreover, a random forest (RF) model was proposed with hyperparameters tuned by beetle antennae search (BAS), aiming at predicting FS and ASR expansion precisely. A large database was established from the experimental results based on 549 samples prepared for the FS test and 183 samples produced for the expansion test. The BAS-RF model presented high correlation coefficients for both FS (0.9545) and ASR (0.9416) data sets, showing much higher accuracy than multiple linear regression and logistic regression. Finally, a sensitivity analysis was conducted to rank the variables based on importance. Apart from the curing time, the particle granularity and content of WG were demonstrated to be the most sensitive variable for FS and expansion, respectively.

Keywords: random forest; beetle antennae search; activation methodology; machine learning; flexural strength

1. Introduction

Sustainable construction involves the creation of a resource-efficient and eco-friendly environment. Construction waste reduction and waste recycling are two essential principles of this practice. Waste glass (WG) is a common urban solid waste, which is hazardous to the environment because of its inert and biodegradable properties. However, WG treatment is expansive, and its reuse is still at the initial stage. Statistically, 11,530 kilotons of WG were generated in the United States in 2010, with only 30% recycled, and approximately 300 tonnes per day were produced in Hong Kong in 2016, with only 10% recycled [1,2].
Therefore, developing a feasible method to cope with the increasing WG content is urgent and essential.

Due to its abundance, low cost, and high stiffness, WG has been used in the construction industry. Previous research studies have shown that WG is a good replacement for sand or cement, serving as a supplementary cementitious material. This is mainly attributed to WG’s high silica content (over 70%), which can react with calcium hydroxide (CH) to generate calcium silica hydrates (C-S-H). Furthermore, glass can alleviate the corrosion of steel bars within reinforced concrete. Therefore, reusing WG in concrete manufacturing is promising in terms of increasing its recycling degree, reducing carbon dioxide emissions caused by cement production, and mitigating the shortage of high-quality sand.

However, the strength property and expansion arising from alkali–silica reaction (ASR) of concrete containing WG are two key points that must be investigated before applying WG. This is mainly due to WG’s chemical and physical properties. Generally, discarded glass cullet from bottles, windows, decorations, etc. has poor geometry, that is, an angular, flat, or elongated shape, leading to poor workability and diminished strength grade [3,4]. In addition, the high silica content of WG will inevitably produce ASR expansion and probably result in structural instability, which is the chief reason for the failed early application of waste glass concrete [5,6]. Therefore, the investigation on ASR expansion and reliable expansion prediction is essential.

To overcome the reduced strength and excessive ASR expansion, researchers made massive efforts to investigate concrete containing WG and proposed many practicable approaches. These include in-depth studies of glass granularity and admixtures. When the glass cullet was milled to less than 300 µm, both the pozzolanic level of waste glass powder (WGP) and the strength of concrete significantly increased [7–9]. Several studies even pointed out the improved pozzolanic ability (compared with fly ash) from ground WG with particle sizes below 100 µm [5,10]. Moreover, the smaller particle sizes of waste glass can mitigate ASR expansion, as demonstrated by many reports [11,12]. Corinaldesi et al. [13] observed improved unconfined compression strength and flexural strength (FS) without obvious macroscopic expansion. Petrella et al. [14] conducted the mechanical test on mortar containing waste porous glass and found the good adhesion of the glass to the cement paste through microstructural observations. Furthermore, the addition of admixtures, such as silica fume, fly ash, lithium compounds, and metakaolin was useful in preventing deleterious ASR expansion [15,16]. Adhikary et al. [17] also illustrated that expanded glass produced by mixing waste glass and expansive agents was effective in prohibiting the ASR expansion.

Previous studies concentrated on the aforementioned aspects in solving the strength and expansion problems, but few reports mentioned the chemical activation of WGP. The possible explanations are the complex chemical reactions and the various types of chemical agents. Additionally, the traditional method of analysis is inadequate in seeking optimal mixture proportions and controlling the error when the variables are multiple. Although multiple linear regression (MLR) and logistic regression (LR) have been proposed, an accurate simulation is still challenging mainly due to the curse of dimensionality and co-linearity susceptibility [18–20]. Therefore, this study aimed to activate WGP using chemical activators and an accurate machine learning (ML) model to predict the FS and ASR expansion of WGP mortars.

Recently, the performance of cementitious materials has been broadly studied using artificial intelligence (AI) techniques. ML models exhibit an excellent generalisation ability and perfect prediction accuracy in coping with nonlinear tasks [21,22]. The artificial neural network (ANN), support vector regression (SVR), and random forest (RF) are three widely used ML models that are effective for employing various construction materials [23,24]. The first two models are standalone, while the latter (RF) is an ensemble model that exhibits less probability of generating overfitting problems. RF also has better tolerance than standalone ML models when outliers or noise exist in the data set [25,26]. Furthermore, the blessing of dimensionality and the central limit theorem partly contribute to the success of the
ensemble models that outperform the individual models. Therefore, the performance of the RF model is expectedly higher than individual models in solving high dimensionality problems [27,28]. As a result, the RF model was chosen for data prediction.

The accuracy of the RF model depends mainly on two hyperparameters: the total number of trees (numTree) and the minimum sample number of a leaf node (minNumLeaf) [29]. The numTree has a remarkable effect on the model’s ability, and the minNumLeaf controls the splitting condition and determines the relationship between various decision trees. Nevertheless, the process of determining the optimal hyperparameters is time consuming and thus inadequate through the traditional selection method, and if time was not the issue, they would work as well [25]. Recently, optimisation algorithms are preferable since they can automatically seek optimal hyperparameters via iterations. Commonly used metaheuristic algorithms include particle swarm optimisation (PSO) [30], genetic algorithm (GA) [31], and firefly algorithm (FA) [32], which are all computationally intensive. The beetle antennae search (BAS) algorithm uses only one beetle to search the optimal hyperparameters instead of the beetle swarm so that it converges fast and significantly reduces calculation time [33,34]. However, BAS is easily trapped into a local optimum as indicated by previous researchers [35,36]. To reduce the possibility of the local optimum, the BAS algorithm with a changeable step size was proposed for the RF hyperparameter adjustment in this study.

This study investigated the impact of the mechanical, chemical, and mechanical–chemical (combined) activation on the FS and ASR expansion of mortars containing WGP. The sand was replaced with WGP with mean particle sizes of 75 μm and 300 μm. The variables were the replacement ratio, the WGP size, and the content and category of chemical activators (sodium sulphate, calcium hydroxide, and sodium hydroxide). A microscopic test was conducted to investigate the activation effect. In total, 549 samples were prepared for the FS test, and 183 samples were produced for the expansion test. The experimental results are presented as the data set to train the highly accurate BAS-RF model. The baseline models (LR and MLR) were also adopted to compare with BAS-RF. In addition, the sensitivity analysis (SA) was performed on the FS and ASR expansion data sets for a ranking of the input variables.

2. Experimental Program

2.1. Materials and Methods

The mean particle sizes of WGP derived from waste glass vessels were 75 μm and 300 μm. Before being crushed and ground, the vessels were cleaned to eliminate labels and taps and then air-dried. Then, the milled WGP was properly reserved in a sealed and dry container. Figure 1 shows the 75 μm and 300 μm WGP, and Table 1 presents the chemical ingredients. The high silicon dioxide content (approximately 74%) demonstrates the excellent potential of WGP as pozzolans [37]. The ordinary Portland cement (with a strength grade of 42.5) was utilised as an essential binder composition, whose physical and chemical indexes are presented in Table 2. Natural sand was used as the filler with over 96% silicon dioxide, and ASTM C778 [38] was used for its gradation before use.

![WGP](image1.png)

(a) 75 μm WGP  (b) 300 μm WGP

Figure 1. The features of WGP of different granularity: (a) 75 μm; (b) 300 μm.
To investigate the activation effects, five variables were considered: the particle size and substitute proportion of WGP, the category and content of the chemical activators, and the curing times. These five variables were set as the features for the ML modelling. Natural sand was replaced with WGP (75 µm and 300 µm) on three levels (10 wt%, 20 wt%, and 30 wt%). The chemical additive comprises a salt activator (sodium sulphate) and alkaline activators (calcium hydroxide and sodium hydroxide). Additionally, the water-to-cement (W/C) and aggregate-to-cement ratios (A/C) were maintained at 0.47 and 2.25, respectively. The following is the detailed activation methodology:

- **Mechanical activation:** By employing a ball mill, a glass cullet was ground into WGP with two particle sizes: 300 µm and 75 µm. Compared to coarse WGP (300 µm), the finer WGP was supposed to acquire better pozzolanic characteristics.

- **Chemical activation:** Sodium hydroxide, calcium hydroxide, and sodium sulphate (anhydrous) were the three agents used to activate WGP and the WGP–cement system. They are all analytically pure (AR) and commercially available. The alkaline activator is composed of 50 wt% sodium hydroxide and 50 wt% calcium hydroxide, and sodium sulphate served as a salt activator. Both activators were jointly applied at 2 wt%, 4 wt%, and 6 wt% of cement. Before their application, sodium sulphate and sodium hydroxide were dissolved in water, while calcium hydroxide was directly mixed with WGP and sand. The mixing time was enough for the thorough dispersion of raw materials as per ASTM C305 [39].

- **Combined activation:** The mechanical–chemical activation integrated the abovementioned mechanical and chemical approaches, where the 300 µm WG was ground to 75 µm WGP, and the chemical activators were utilised in the meantime.

In total, 60 mixes with one control group are summarised in Table 3, where the WG, sodium sulphate, and alkali activators are expressed as G, S, and H, respectively. The particle sizes of WGP are represented as the numbers 75 and 300 without the unit. The numbers 10, 20, and 30 represent the replacement ratios of WGP, i.e., 10%, 20%, and 30%, respectively. The numbers 2, 4, 6 represent the chemical activators’ ratios of 2%, 4%, and 6%, respectively.
Table 3. The mix proportions of WGP cementitious composites.

| Specimen ID | Cement (g) | Natural Sand (g) | Water (g) | WGP (g) | Na$_2$SO$_4$ (g) | Alkali (g) |
|-------------|------------|------------------|----------|---------|-----------------|------------|
| C (Control Sample) | 450 | 1012.5 | 211.5 | 0 | 0 | 0 |
| Waste Glass Powder (75 µm) |
| 75G10 | 450 | 911.25 | 211.5 | 101.25 | 0 | 0 |
| 75G10S2H2 | 450 | 911.25 | 211.5 | 101.25 | 9 | 9 |
| 75G10S2H4 | 450 | 911.25 | 211.5 | 101.25 | 9 | 18 |
| 75G10S2H6 | 450 | 911.25 | 211.5 | 101.25 | 9 | 27 |
| 75G10S4H2 | 450 | 911.25 | 211.5 | 101.25 | 18 | 9 |
| 75G10S4H4 | 450 | 911.25 | 211.5 | 101.25 | 18 | 18 |
| 75G10S4H6 | 450 | 911.25 | 211.5 | 101.25 | 18 | 27 |
| 75G10S6H2 | 450 | 911.25 | 211.5 | 101.25 | 27 | 9 |
| 75G10S6H4 | 450 | 911.25 | 211.5 | 101.25 | 27 | 18 |
| 75G10S6H6 | 450 | 911.25 | 211.5 | 101.25 | 27 | 27 |
| 75G20 | 450 | 810 | 211.5 | 202.5 | 0 | 0 |
| 75G20S2H2 | 450 | 810 | 211.5 | 202.5 | 9 | 9 |
| 75G20S2H4 | 450 | 810 | 211.5 | 202.5 | 9 | 18 |
| 75G20S2H6 | 450 | 810 | 211.5 | 202.5 | 9 | 27 |
| 75G20S4H2 | 450 | 810 | 211.5 | 202.5 | 18 | 9 |
| 75G20S4H4 | 450 | 810 | 211.5 | 202.5 | 18 | 18 |
| 75G20S4H6 | 450 | 810 | 211.5 | 202.5 | 18 | 27 |
| 75G20S6H2 | 450 | 810 | 211.5 | 202.5 | 27 | 9 |
| 75G20S6H4 | 450 | 810 | 211.5 | 202.5 | 27 | 18 |
| 75G20S6H6 | 450 | 810 | 211.5 | 202.5 | 27 | 27 |
| Waste Glass Powder (300 µm) |
| 75G30 | 450 | 708.75 | 211.5 | 303.75 | 0 | 0 |
| 75G30S2H2 | 450 | 708.75 | 211.5 | 303.75 | 9 | 9 |
| 75G30S2H4 | 450 | 708.75 | 211.5 | 303.75 | 9 | 18 |
| 75G30S2H6 | 450 | 708.75 | 211.5 | 303.75 | 9 | 27 |
| 75G30S4H2 | 450 | 708.75 | 211.5 | 303.75 | 18 | 9 |
| 75G30S4H4 | 450 | 708.75 | 211.5 | 303.75 | 18 | 18 |
| 75G30S4H6 | 450 | 708.75 | 211.5 | 303.75 | 18 | 27 |
| 75G30S6H2 | 450 | 708.75 | 211.5 | 303.75 | 27 | 9 |
| 75G30S6H4 | 450 | 708.75 | 211.5 | 303.75 | 27 | 18 |
| 75G30S6H6 | 450 | 708.75 | 211.5 | 303.75 | 27 | 27 |
| 300G10 | 450 | 911.25 | 211.5 | 101.25 | 0 | 0 |
| 300G10S2H2 | 450 | 911.25 | 211.5 | 101.25 | 9 | 9 |
| 300G10S2H4 | 450 | 911.25 | 211.5 | 101.25 | 9 | 18 |
| 300G10S2H6 | 450 | 911.25 | 211.5 | 101.25 | 9 | 27 |
| 300G10S4H2 | 450 | 911.25 | 211.5 | 101.25 | 18 | 9 |
| 300G10S4H4 | 450 | 911.25 | 211.5 | 101.25 | 18 | 18 |
| 300G10S4H6 | 450 | 911.25 | 211.5 | 101.25 | 18 | 27 |
| 300G10S6H2 | 450 | 911.25 | 211.5 | 101.25 | 27 | 9 |
| 300G10S6H4 | 450 | 911.25 | 211.5 | 101.25 | 27 | 18 |
| 300G10S6H6 | 450 | 911.25 | 211.5 | 101.25 | 27 | 27 |
| 300G20 | 450 | 810 | 211.5 | 202.5 | 0 | 0 |
| 300G20S2H2 | 450 | 810 | 211.5 | 202.5 | 9 | 9 |
| 300G20S2H4 | 450 | 810 | 211.5 | 202.5 | 9 | 18 |
| 300G20S2H6 | 450 | 810 | 211.5 | 202.5 | 9 | 27 |
| 300G20S4H2 | 450 | 810 | 211.5 | 202.5 | 18 | 9 |
| 300G20S4H4 | 450 | 810 | 211.5 | 202.5 | 18 | 18 |
| 300G20S4H6 | 450 | 810 | 211.5 | 202.5 | 18 | 27 |
| 300G20S6H2 | 450 | 810 | 211.5 | 202.5 | 27 | 9 |
| 300G20S6H4 | 450 | 810 | 211.5 | 202.5 | 27 | 18 |
| 300G20S6H6 | 450 | 810 | 211.5 | 202.5 | 27 | 27 |
| 300G30 | 450 | 708.75 | 211.5 | 303.75 | 0 | 0 |
| 300G30S2H2 | 450 | 708.75 | 211.5 | 303.75 | 9 | 9 |
| 300G30S2H4 | 450 | 708.75 | 211.5 | 303.75 | 9 | 18 |
| 300G30S2H6 | 450 | 708.75 | 211.5 | 303.75 | 9 | 27 |
| 300G30S4H2 | 450 | 708.75 | 211.5 | 303.75 | 18 | 9 |
| 300G30S4H4 | 450 | 708.75 | 211.5 | 303.75 | 18 | 18 |
| 300G30S4H6 | 450 | 708.75 | 211.5 | 303.75 | 18 | 27 |
| 300G30S6H2 | 450 | 708.75 | 211.5 | 303.75 | 27 | 9 |
| 300G30S6H4 | 450 | 708.75 | 211.5 | 303.75 | 27 | 18 |
| 300G30S6H6 | 450 | 708.75 | 211.5 | 303.75 | 27 | 27 |
2.2. Mechanical Test

The FSs at 7, 14, and 28 curing times were tested for each mix of mortar containing WGP. Three parallel specimens were cast and the mean values were calculated as the ultimate results after eliminating the outliers. The FS samples were prepared in a prismatic shape (40 × 40 × 160 mm), complying with ASTM C348 [40]. After casting, the mortar samples with moulds were transferred to a wet closet at 20 ± 1 °C temperature and 95 ± 5% humidity for 24 h. Then, the samples were separated from the moulds and stored in saturated lime water until the curing time ended. A three-point bending apparatus was fabricated at a steady loading level of 0.03 MPa/s and the flexural strength $f_s$ (MPa) was formulated in Equation (1). The results of mechanical test are summarised in the Appendix A.

$$f_s = \frac{3FL}{2bh^2}$$  \hspace{1cm} (1)

where $F$ is the fracture surcharge (N); $L$, $h$, and $b$ are the length, height, and width of the sample (mm), respectively.

2.3. Alkali–Silica Reaction

The ASR experiment was conducted per ASTM C1260 [41] to estimate the risk of detrimental expansion. For each mix, the average longitudinal change of three identical bar samples (25 × 25 × 280 mm) was determined after 2, 4, 7, 10, and 14 days. The effective length of the specimen was 260 mm, which was the length between two steel stud gauges, as shown in Figure 2. The prepared samples are shown in Figure 3. After casting, they were stored in the moisture closet for 24 h and were subsequently immersed in water (80 °C) for another 24 h. The initial lengths $L_0$ of the samples (accurate to 0.002 mm) were measured through a length comparator, and then specimens were transferred to a 1 N 80 °C NaOH solution. The longitudinal length of the sample at day $x$ is symbolised by $L_x$, and the expansion proportion $e_x$ can be determined by Equation (2). The deleterious expansion is negligible if the expansion ratio at 14 days is less than 0.1%. The results of ASR test are summarised in the Appendix B.

$$e_x = \frac{L_x - L_0}{260} \times 100\%$$  \hspace{1cm} (2)

Figure 2. Schematic figure of ASR expansion test.
Figure 3. Bar specimens used in ASR expansion test.

2.4. Scanning Electron Microscopy

To investigate the microscopic influence of chemical activators on WGP and the bonding ability of WGP with hydration products, scanning electron microscopy (SEM) was employed as a supplementary test. The chemically activated WGP samples were fabricated by immersing them into the water that dissolved the alkali and sodium sulphate for 7 days. The mortar specimens for the SEM experiment were derived from the sample fragments after conducting the FS test.

3. Machine Learning Models

The ML models utilised in this study are RF, LR, and MLR. In this section, the RF model is elaborated, followed by the baseline models (LR, MLR). The BAS algorithm and 10-fold cross-validation (CV) are subsequently explained with the ability to optimise the hyperparameters of RF and increasing the prediction performance of ML, respectively. The model evaluation index and variable sensitivity analysis are finally demonstrated.

3.1. Random Forest Model

To acquire more reliable output, random forest generates hundreds of decision trees (RTs) with their own regression functions. RT is a nonparametric model which consists of a root node, decision nodes, and leaf nodes. The training set is represented as $R_n$ shown in Equation (3) where $X$ and $Y$ are the input vector with $m$ features ($X = \{x_1, x_2, \ldots, x_m\}$) and the output scalar, respectively. In this study, $R_n$ represents the FS and ASR datasets. The $X$ and $Y$ indicate the input vector with five features and the outputs (FS, ASR), respectively. Each sample in the training set will be evaluated by the decision nodes using a split function. Then, the sample will be passed to different branches until the leaf node is reached. The tree is stopped when the minimum sample number of a leaf node is achieved.

During the training process of each RT, $n$ samples from the training set $R_n$ are randomly sampled without replacement ($1/n$ possibility for each sample to be selected at each time). This sample collecting process is called ‘bootstrap’, and the corresponding sample set is represented as $R_n^b$. Subsequently, the samples of $R_n^b$ are split from the root node to the leaf node with each node applying its own split function. At the end of this training process, the prediction function $\hat{\delta}(X, R_n^b)$ is established over $R_n^b$.

As mentioned before, the RF is an extension of RT constructing numerous RTs. A ‘bagging’ method is applied to integrate all the results derived from these RTs and utilises the average value as the final output [42]. The bagging technique is proposed by Breiman [43], which effectively reduces the prediction variance to improve prediction performance. The
RF algorithm is described in Figure 4 in which RF comprises \( k \) de-correlated RTs so that \( k \) prediction functions \( \hat{a}(X, R^0_n) \), where \( k = 1, 2, \ldots, k \), will be constructed. The symbol \( \theta_k \) represents independently distributed random vector to represent different RTs. Finally, the RF produces \( k \) outputs \( \{ \hat{Y}_1, \hat{Y}_2, \ldots, \hat{Y}_k \} \) corresponding to each RT. The ultimate prediction \( Y \) is achieved by averaging these outputs as shown in Equation (4).

\[
R_n = \{ (X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n) \}, \quad X \in \mathbb{R}^m, Y \in \mathbb{R}.
\]

\[
Y = \frac{1}{k} \sum_{i=1}^{k} \hat{Y}_i = \frac{1}{k} \sum_{i=1}^{k} \hat{a}(X, R^0_n)
\]

**Figure 4.** Construction of an RF model.

### 3.2. Baseline Models

Lasso regression is a type of linear regression method using shrinkage theory that can address high levels of multicollinearity problems [44,45]. However, LR and MLR models are more popular than Lasso regression in solving regression problems in the construction field [46,47]. Therefore, these two baseline models (LR and MLR) are proposed to compare with the BAS-RF model and assess their prediction discrepancy.

### 3.3. Beetle Antennae Search (BAS)

To automatically seek the optimal hyperparameters of the RF model, the BAS algorithm is proposed, which is derived from the foraging behaviour of the longhorn beetle [48,49]. The beetle can continuously change the moving orientation according to its two antennae that can perceive the odour concentration. In the BAS algorithm, we use \( x_l \) and \( x_r \) to symbolise the location of the left and right antennae. Their placements at the \( i^{th} \) time instant can be given by

\[
x_l^i = x_l^{i-1} + \delta^i b \text{sign} \left( f \left( x_l^{i-1} \right) - f \left( x_r^{i-1} \right) \right)
\]

where \( b \) is a random vector and can be written in Equation (6).

\[
b = \frac{\text{rand}(k,1)}{\| \text{rand}(k,1) \|}
\]

where \( \text{rand}(k,1) \) is a random function having \( k \) dimensions. The following equations show the location vector of the beetle, the updated antennae length, and the step size.

\[
x_l^i = x_l^{i-1} + \delta^i b \text{sign} \left( f \left( x_l^{i-1} \right) - f \left( x_r^{i-1} \right) \right)
\]
where \( \delta \) means the step length; \( f(x) \) represents fitness function; \( \text{sign}(\cdot) \) is a sign function that extracts the sign of a real number.

### 3.4. The 10-Fold Cross-Validation Process

Two hyperparameters of the RF model need to be adjusted, which are \( \text{numTree} \) and \( \text{minNumLeaf} \). To eliminate the overfitting problems caused by a limited database, a 10-fold cross-validation method was utilised, which is frequently used in predicting cementitious materials performance [47,50]. Meanwhile, all the data can be used for training and testing, giving a fair and comprehensive evaluation metric, although the database is not large. Therefore, the small dataset limitation is supposed to be eliminated. During the process of CV, the data set is firstly randomly separated into two parts: the test group (30%) and the training group (70%) [51]. Secondly, the training group is divided into 10 folds among which the 9 folds are applied to develop the RF model and the rest is for performance validation [52,53]. During the modelling process, the RF hyperparameters are tuned by the BAS algorithm through 50 iterations. Additionally, the root means square error (RMSE) is obtained when finishing validating. This process repeats 10 times to compare the validation outcome. Ultimately, the trained model with the minimum RSME and optimal hyperparameters was used to predict the FS and ASR expansion in this study. The procedure of RF model training by 10-fold CV and BAS is shown in Figure 5.

**Figure 5.** RF model training by 10-fold CV and BAS.

### 3.5. Performance Evaluation

The RMSE and correlation coefficient \( (R) \) are two evaluation indexes to estimate the accuracy of various ML models. The definitions are as follows:

\[
RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i^* - y_i)^2}
\]  

(10)

\[
R = \frac{\sum_{i=1}^{N} (y_i^* - \bar{y})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{N} (y_i^* - \bar{y})^2 \sqrt{\sum_{i=1}^{N} (y_i - \bar{y})^2}}}
\]  

(11)
where \( n \) represents the quantity of the data specimens; \( y_i^* \) is the predicted output by the ML models; \( y_i \) is the actual output in the data set; \( \bar{y}^* \) and \( \bar{y} \) are the mean values of the predicted and actual values, separately.

### 3.6. Variable Significance Determination

An approach based upon sensitivity analysis (SA) was used to investigate the connection between variables and outcomes. Within the range of input variables, this method can assess the impact on the output by changing the input values [54,55]. The beginning procedure is to design input and output variables, followed by evaluating each input variable with all the other variables constant. The SA comprises global sensitivity analysis (GSA) and local sensitivity analysis (LSA), but LSA cannot be used to search uncertainties. In contrast, GSA can simultaneously assess all input variables and therefore is applied in this study. Finally, importance sequences (0 to 100%) are visualised through bar charts [56].

The following equations show a gradient metric to estimate the resulting change of the output and the relative importance formulation [56].

\[
g_\varepsilon = \frac{1}{L} \sum_{j=2}^{L} \frac{|\hat{y}_{\varepsilon,j} - \hat{y}_{\varepsilon,j-1}|}{L - 1} \quad (12)
\]

\[
R_\varepsilon = g_\varepsilon / \sum_{i=1}^{L} g_i \quad (13)
\]

where \( \varepsilon \) is the analysed input variable; \( \hat{y}_{\varepsilon,j} \) represents the susceptibility reaction indicator for \( x_{\varepsilon,j} \); \( R_\varepsilon \) is the relative importance of the variable.

### 4. Results and Discussion

#### 4.1. Results of the Laboratory Experiments

##### 4.1.1. Results of the Flexural Strength Test

Figure 6 shows the FS values of mortar samples containing different WGP substituting ratios without adding chemical agents at 7, 14, and 28 days. Lower FS was observed in specimens containing 300 \( \mu m \) WGP, which agrees with previous findings that coarse glass adversely affected mechanical characteristics [1,57]. In contrast, the mortar specimens containing 75 \( \mu m \) WGP exhibited improved FS, compared to both 300 \( \mu m \) WGP samples and the control one. This phenomenon illustrates the positive effect of mechanical activation in increasing FS. The 10% 75 \( \mu m \) WG proportion showed the highest strength at 9.7 MPa (28 days), which was 26.63% higher than that of the control sample. Moreover, the FS of the sample containing 30% 75 \( \mu m \) WGP was 7.6 MPa, which almost reached the same strength level as the ordinary mortar sample. This is mainly attributed to the bonding strength arising from WGP’s pozzolanic reaction [11,58,59]. When glass’s particle granularity shrank through physical grinding, its stable silica tetrahedron structure would be destroyed, leading to reduced crystallisation and increased reactivity. Meanwhile, the finer WGP had a larger specific surface area and simultaneously compacted the mortar structure through evenly distributed in the pores of the mortar. Therefore, it is effective to increase the FS of WGP mortars by applying a mechanical approach.

Figure 7 compares the 28-day FS results of the mortar samples containing 300 \( \mu m \) and 75 \( \mu m \) WGP (10%, 20%, and 30%) under the chemical activation. When the WGP particle size was 300 \( \mu m \), the FS increase was only observed in samples containing activated WGP (2% Na\(_2\)SO\(_4\) and 2% alkali), compared to mortars with nonactivated WGP. Meanwhile, the FS in all the 300 \( \mu m \) WGP mortars was less than that in the control sample, illustrating the limited chemical activation effect on coarse glass particles. The opposite phenomenon was observed when the WGP size was mechanically ground into 75 \( \mu m \). Figure 7c shows the highest FS value (around 9 MPa) on the mortar sample with 30% WGP (75 \( \mu m \)) under the treatment of 2% Na\(_2\)SO\(_4\) and 2% alkali. It was both higher than the 30% nonactivated WGP sample (7.60 MPa) and the normal sample (7.66 MPa), indicating the positive efficacy of the
mechanical–chemical activation. However, the FS was reduced provided that the 75 μm activated WGP content was 10%, as shown in Figure 7a. This is mainly due to the excessive ASR expansion that exceeded the ASTM threshold (0.1%) shown in following chapters.

Figure 6. The FS of mortar containing WGP with different proportions by mechanical activation at different curing times.

The Na$_2$SO$_4$ and alkali effect on the WGP–cement system is analogous to that on fly ash–cement system considering the slow pozzolanic reaction and similar chemical constituents for WGP and fly ash. According to the previous findings, the Na$_2$SO$_4$ reacts with Ca(OH)$_2$ to generate gypsum and NaOH [60,61]. The gypsum further reacts with the aluminia in cement to generate ettringite (Aft), and NaOH participates in the reaction with Ca(OH)$_2$ and WGP (or fly ash) to produce the additional gels [62,63]. This results in more hydration products compacting the WGP mortar structure and improving the flexural strength. In addition, the Alite (C$_3$S) hydration has been verified to be accelerated under the high concentration of dissolved sulphate ions [60]. Therefore, more calcium silicate hydrates and calcium hydroxide will be generated to further increase mechanical strength.

Regarding the alkali (NaOH and Ca(OH)$_2$) effect, it has been verified to effectivly depolymerise WGP structure by destroying the chemical bond between the oxygen atom and silicon [64,65]. Therefore, the WGP stable Silica tetrahedron units can be broken to accelerate the silica dissolution and WGP pozzolanic reaction, as illustrated by many researchers [66,67]. However, the results in Figure 7 also indicated the negative effect of both Na$_2$SO$_4$ and alkali when their contents were over 2%. This was in agreement with the previous investigations that excessive Na$_2$SO$_4$ and alkali would lead to numerous Aft generation and heterogeneous gel production, respectively [64,68]. Therefore, the loose structure can be ultimately formed diminishing the flexural strength. Moreover, the excessive alkali content also increases the risk of detrimental ASR expansion. From the FS test results, the optimal content of chemical agents is 2% Na$_2$SO$_4$ and 2% alkali.
Figure 7. The 28-day FS of mortar containing (a) 10%, (b) 20%, and (c) 30% WGP by chemical activation.
4.1.2. Results of the Alkali–Silica Activation Test

Figure 8 shows the increase in the ASR expansion with curing time. The expansion kept increasing with the rise in the WGP ratio. The 14-day ASR expansion of all mortars containing 300 μm WGP was larger than the expansion of the control specimens. This demonstrates the negative effect of coarse glass powder, which is consistent with the previous investigations [69,70]. In contrast, the mortar sample containing 10% 75 μm WGP showed the lowest expansion value (0.0192% at 14 days), which was much less than the control sample and the ASTM threshold. This resulted from the pozzolanic reaction of WGP, which is prone to generating gels with nonswelling properties [71,72]. However, the excessive ASR expansion was obvious when the WGP (75 μm) ratio was increased to 30%. This phenomenon disagreed with the previous finding that fine glass particle was harmless to the ASR expansion. Du et al. [69] explained that this may be attributed to the microcracking of the glass powder during the grinding process. Although high WGP content can cause detrimental expansion, mechanical grinding’s efficacy in mitigating ASR expansion has been verified.

Figure 9 depicts the impact of chemical activation on 14-day ASR results of samples with different WGP particle sizes and contents. When the WGP ratios were 10% and 20%, the chemical activator showed adverse effects because a larger expansion appeared on chemically excited samples. However, this negative effect turned out to be positive when the WGP ratio was increased to 30%, as shown in Figure 9c. The ASR expansion was 0.0654% for 30% WGP samples activated by 2% Na₂SO₄ and 2% alkali, which was 54% smaller than that of specimen 75G30. This might be because the alkali activator increased the concentration of calcium ions, thus generating fewer swelling gels [66,73]. Regarding the chemical activator’s content, the relationship between it and ASR expansion was not obvious, and therefore, ML models were proposed, as discussed in the next section. Generally, chemical activation was feasible in mitigating the detrimental ASR expansion only for mortars with high WGP content. Specifically, the mitigation effect of chemical activator on ASR expansion mainly depended on the WGP content other than the activator’s content. Combined with the FS results, mortars containing 30% 75 μm WGP activated by 2% Na₂SO₄ and 2% alkali can achieve improved strength and satisfactory potential for ASR expansion.
Figure 9. The 14-day ASR values of bar samples containing (a) 10%, (b) 20%, and (c) 30% chemically activated WGP.
4.1.3. Results of SEM

Figure 10 shows the microstructures of different WGP and mortar samples, exploring the chemical activation’s effect. The relatively smooth surface of the nonactivated WGP was in striking contrast with the eroded surface shown in Figure 10c. This phenomenon indicates the susceptibility of the WGP to chemical activators. Moreover, more hydrates and finer fissures were revealed in the WGP mortar sample activated by 2% alkali and 2% Na$_2$SO$_4$, compared with the nonactivated one. Figure 10d shows that fewer calcium hydroxide (CH) crystals were detected than in the sample without chemical activation, indicating a more intense pozzolanic reaction. Therefore, the chemical agents promote the pozzolanic activation of WGP and simultaneously increase its mechanical property, as described before, if the activators’ content is moderate.

![Figure 10. SEM micrographs of (a) 75 μm WGP, (b) mortar-75G10, (c) pretreated 75 μm WGP by 2% alkali and 2% Na$_2$SO$_4$, and (d) mortar-75G10S2H2.](image)

4.2. Modelling Results

4.2.1. Hyperparameter Tuning

By using BAS and 10-fold CV, the optimal hyperparameters can be obtained from the fold having the minimum RMSE. As shown in Figure 11, the first and fourth folds achieved the minimum RMSE in the process of FS and ASR modelling. The RMSE converged during the 50 iterations, illustrating the success of hyperparameter tuning and model establishment. Finally, the optimal hyperparameters chosen for FS and ASR datasets were both minNumleaf = 1 and numTree = 87.
4.2.2. Performance of BAS-RF for FS and ASR Expansion Modelling

The capability of the RF model with adjusted hyperparameters was verified by assessing the predictive precision of the test group. In Figure 12, the predicted and actual FS and ASR values in the training and test groups are presented. The relationship between the predicted and actual outcomes was estimated by calculating the \( \text{RMSE} \) and correlation coefficient. Apart from minor \( \text{RMSE} \) values, high correlation coefficients were observed for both training (FS: 0.9841, ASR: 0.9582) and test sets (FS: 0.9545, ASR: 0.9416). Therefore, the prediction performance of the ML models was accurate and reliable. Furthermore, the \( \text{RMSE}/R \) values of the training set and test set were close illustrating that no overfitting problem existed.

![Figure 11. RSME values from 10 validation sets for (a) FS and (b) ASR modelling.](image-url)
4.2.3. Comparison of Two Baseline Models with the BAS-RF

The precision of the BAS-RF model, compared with the other two (LR and MLR), is shown in Figure 13 through boxplots and Taylor diagrams. The difference between the predicted and actual sample values is indicated in the boxplot. In Figure 13a, the RF model had a lower median value (the red line) and a more condensed interquartile range (the space between the upper and lower blue lines). This phenomenon indicated a lower prediction error than the other two baseline models. In addition, the upper limit of the RF was lower than the LR and MLR, although one outlier was observed, illustrating the high accuracy of the RF model. In Figure 13b, the RF model was also more accurate in predicting ASR values than LR and MLR because of its condensed interquartile range although several outliers appeared. Moreover, three model evaluation indices (standard deviation, RMSE, and R) are integrated into the polar coordinates, as shown in Figure 13c,d. The two RF models were both in the closest position to the “actual” points with the uppermost R-value, minimum RMSE, and lowest standard deviation values. Owing to the highest prediction accuracy and lowest error among the three ML models, the BAS-RF model is the most suitable to predict the FS and ASR values of WGP modified mortar.
4.3. Variable Significance for FS and ASR Expansion

The effects of the variables on the FS and ASR results were quantified as the importance ratio presented in Figure 14. The curing time is the most significant factor for both FS and ASR expansion. The WGP particle size was the second important variable for FS (26%), thus remarkably affecting the mechanical strength of mortars containing WGP. This was followed by the alkali content (18%) and the WGP replacement ratio (12%). Further, Na₂SO₄ appeared less important than alkali, which agrees with the experimental findings. For the ASR expansion, the WGP replacement ratio became the most significant factor (16%) except for the curing time. This agreed with the experimental results that ASR expansion significantly depended on the WGP replacement ratio other than the activator’s content. Moreover, the alkali content was less important than Na₂SO₄, which is reasonable since the 1 N NaOH solution was used to immerse the samples. In conclusion, the importance measure provides a quantitative analysis of input variables, indicating that the WGP’s particle size and replacement ratio are the most crucial parameters (except curing time) for FS and ASR, respectively.
5. Conclusions

In this study, the characteristics of mortars containing WGP were investigated by conducting FS and ASR expansion tests. Based on the experimental data set, three ML models were applied to simulate the FS and expansion values. The prediction results were consistent with the actual figures and the essential conclusions were described as follows:

1. WGP’s mechanical grinding significantly improved the FS of WGP mortars. The chemical activation was only effective when the amounts of the chemical agents were appropriate. The combined activation exhibited the most remarkable efficacy; the FS of the sample containing 30% WGP that underwent the combined activation method was 8.97 MPa (18% higher than the sample subjected to mechanical excitation only).

2. Mechanical activation mitigated ASR expansion, and chemical activation was also feasible when the WGP content was 30%. The ASR expansion was 0.0654% (54% lower than the nonactivated one) for the sample that had 30% of WGP with combined activation. This illustrates the effectiveness of combined activation. The SEM results also verified its efficacy which improved the pozzolanic activity of WGP and concurrently compacted the mortars’ structure.

3. The accuracy of the BAS-RF model in predicting FS and ASR expansion was reflected in the high $R$ values (0.9545 for FS and 0.9416 for ASR expansion). Compared with the other two baseline models (LR and MLR), the BAS-RF model obtained higher $R$ values and fewer $RMSE$ results, showing that both FS and ASR data sets had better properties. The predicted results simulated by the BAS-RF model agreed with the experimental outcomes.

4. The variable significance ranking showed that WGP’s particle size and replacement ratio were the most essential factors (except the curing time) for FS and ASR expansion, respectively. The results also agreed with the experimental findings.

In the future, the activated WGP incorporated 3D-printed concrete and alkali-activated concrete will be investigated. Regarding the ML research, a more comprehensive database must be constructed to increase the model generalisability. The evolved ML models with improved applicability, accuracy, and efficiency should also be developed. Furthermore, it is crucial to investigate more variables, such as glass types, chemical activator categories, and admixtures.
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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

Table A1. The experimental results of 75 µm WGP mortar samples.

| ID   | Flexural Strength (MPa) | ASR Expansion (%) |
|------|------------------------|-------------------|
|      | 7 d  | 14 d  | 28 d  | 0 d   | 2 d   | 4 d   | 7 d   | 10 d  | 14 d  |
| C    | 5.40 | 7.35  | 7.66  | 0     | 0.0196| 0.0225| 0.0308| 0.0346| 0.0462|
| 75G10| 5.64 | 7.64  | 9.70  | 0     | 0.0066| 0.0077| 0.0156| 0.0192| 0.0192|
| 75G10S2H2 | 6.12 | 7.82  | 8.79  | 0     | 0.0346| 0.0385| 0.0519| 0.0692| 0.1038|
| 75G10S2H4 | 5.46 | 7.14  | 8.02  | 0     | 0.0154| 0.0214| 0.0315| 0.0577| 0.0731|
| 75G10S2H6 | 4.66 | 5.54  | 6.57  | 0     | 0.0246| 0.0308| 0.0446| 0.0538| 0.0808|
| 75G10S4H2 | 5.87 | 7.26  | 7.95  | 0     | 0.0231| 0.0292| 0.0538| 0.0984| 0.1430|
| 75G10S4H4 | 5.41 | 6.13  | 7.02  | 0     | 0.0154| 0.0254| 0.0538| 0.0808| 0.1308|
| 75G10S4H6 | 4.19 | 5.60  | 6.00  | 0     | 0.0100| 0.0231| 0.0615| 0.0885| 0.1160|
| 75G10S6H2 | 5.54 | 7.10  | 7.80  | 0     | 0.0038| 0.0115| 0.0462| 0.0846| 0.1192|
| 75G10S6H4 | 5.65 | 6.45  | 7.62  | 0     | 0.0085| 0.0231| 0.0615| 0.1077| 0.1385|
| 75G10S6H6 | 4.60 | 5.56  | 7.18  | 0     | 0.0046| 0.0247| 0.0462| 0.0810| 0.1000|
| 75G20 | 4.46 | 6.02  | 6.98  | 0     | 0.0075| 0.0138| 0.0308| 0.0423| 0.0462|
| 75G20S2H2 | 5.68 | 7.50  | 7.98  | 0     | 0.0157| 0.0346| 0.0385| 0.0538| 0.0692|
| 75G20S2H4 | 5.02 | 6.45  | 7.17  | 0     | 0.0200| 0.0386| 0.0465| 0.0612| 0.0808|
| 75G20S2H6 | 4.26 | 5.95  | 6.63  | 0     | 0.0538| 0.0577| 0.0713| 0.0831| 0.1115|
| 75G20S4H2 | 5.45 | 6.95  | 7.86  | 0     | 0.0346| 0.0538| 0.0615| 0.0756| 0.1000|
| 75G20S4H4 | 4.85 | 6.85  | 7.43  | 0     | 0.0385| 0.0615| 0.0885| 0.1038| 0.1166|
| 75G20S4H6 | 4.36 | 5.90  | 6.11  | 0     | 0.0421| 0.0731| 0.0885| 0.1077| 0.1055|
| 75G20S6H2 | 4.69 | 6.24  | 6.76  | 0     | 0.0077| 0.0192| 0.0500| 0.0650| 0.0846|
| 75G20S6H4 | 4.35 | 6.03  | 7.01  | 0     | 0.0154| 0.0260| 0.0423| 0.0462| 0.0577|
| 75G20S6H6 | 4.16 | 6.00  | 6.73  | 0     | 0.0385| 0.0846| 0.0962| 0.1000| 0.1115|
| 75G30 | 4.96 | 6.85  | 7.60  | 0     | 0.0462| 0.0692| 0.1086| 0.1192| 0.1423|
| 75G30S2H2 | 6.15 | 7.65  | 8.97  | 0     | 0.0154| 0.0200| 0.0269| 0.0500| 0.0654|
| 75G30S2H4 | 5.46 | 6.86  | 8.30  | 0     | 0.0077| 0.0085| 0.0154| 0.0231| 0.0385|
| 75G30S2H6 | 4.65 | 5.55  | 7.00  | 0     | 0.0154| 0.0192| 0.0231| 0.0269| 0.0423|
| 75G30S4H2 | 4.95 | 6.65  | 6.93  | 0     | 0.0192| 0.0288| 0.0346| 0.0427| 0.0462|
| 75G30S4H4 | 4.95 | 6.25  | 7.20  | 0     | 0.0346| 0.0538| 0.0577| 0.0615| 0.0731|
| 75G30S4H6 | 4.02 | 4.95  | 5.96  | 0     | 0.0216| 0.0386| 0.0462| 0.0538| 0.0577|
| 75G30S6H2 | 4.95 | 6.06  | 6.92  | 0     | 0.0208| 0.0269| 0.0346| 0.0513| 0.0615|
| 75G30S6H4 | 4.85 | 5.85  | 7.07  | 0     | 0.0154| 0.0346| 0.0486| 0.0692| 0.0808|
| 75G30S6H6 | 5.19 | 5.86  | 6.63  | 0     | 0.0268| 0.0346| 0.0462| 0.0538| 0.0652|
## Appendix B

### Table A2. The experimental results of 300 µm WGP mortar samples.

| ID    | Flexural Strength (MPa) | ASR Expansion (%) |
|-------|------------------------|-------------------|
|       | 7 d | 14 d | 28 d | 0 d | 2 d | 4 d | 7 d | 10 d | 14 d |
| 300G10 |     |      |      | 4.85 | 7.06 | 0.007 | 0.015 | 0.033 | 0.041 | 0.051 |
| 300G10S2H2 | 5.55 | 6.37 | 7.36 | 0.027 | 0.046 | 0.057 | 0.095 | 0.126 |
| 300G10S2H4 | 4.59 | 5.78 | 6.82 | 0.016 | 0.025 | 0.037 | 0.066 | 0.083 |
| 300G10S2H6 | 4.01 | 4.54 | 5.65 | 0.025 | 0.034 | 0.062 | 0.058 | 0.091 |
| 300G10S4H2 | 4.71 | 5.08 | 5.90 | 0.018 | 0.028 | 0.072 | 0.109 | 0.144 |
| 300G10S4H4 | 3.81 | 4.54 | 4.86 | 0.011 | 0.026 | 0.076 | 0.096 | 0.140 |
| 300G10S4H6 | 3.31 | 4.50 | 4.51 | 0.005 | 0.035 | 0.063 | 0.093 | 0.108 |
| 300G10S6H2 | 3.35 | 4.45 | 4.67 | 0.039 | 0.048 | 0.060 | 0.086 | 0.107 |
| 300G10S6H4 | 3.25 | 4.17 | 5.03 | 0.026 | 0.062 | 0.084 | 0.122 | 0.145 |
| 300G10S6H6 | 3.63 | 4.37 | 4.78 | 0.050 | 0.060 | 0.080 | 0.093 | 0.099 |
| 300G20 |     |      |      | 4.26 | 5.67 | 6.35 | 0.021 | 0.034 | 0.062 | 0.070 | 0.085 |
| 300G20S2H2 | 4.29 | 5.84 | 6.49 | 0.029 | 0.038 | 0.055 | 0.079 | 0.089 |
| 300G20S2H4 | 3.71 | 4.84 | 5.81 | 0.021 | 0.050 | 0.056 | 0.080 | 0.092 |
| 300G20S2H6 | 3.45 | 4.52 | 5.71 | 0.059 | 0.065 | 0.082 | 0.108 | 0.128 |
| 300G20S4H2 | 4.14 | 5.18 | 6.45 | 0.044 | 0.060 | 0.067 | 0.092 | 0.114 |
| 300G20S4H4 | 3.83 | 5.25 | 6.02 | 0.049 | 0.077 | 0.104 | 0.134 | 0.126 |
| 300G20S4H6 | 3.36 | 4.71 | 5.61 | 0.008 | 0.021 | 0.055 | 0.081 | 0.097 |
| 300G20S6H2 | 3.45 | 4.99 | 5.65 | 0.017 | 0.028 | 0.049 | 0.061 | 0.072 |
| 300G20S6H4 | 3.31 | 4.50 | 5.61 | 0.042 | 0.113 | 0.125 | 0.129 | 0.137 |
| 300G20S6H6 | 3.24 | 4.74 | 5.29 | 0.041 | 0.076 | 0.086 | 0.130 | 0.144 |
| 300G30 |     |      |      | 4.06 | 5.13 | 6.10 | 0.039 | 0.053 | 0.086 | 0.113 | 0.120 |
| 300G30S2H2 | 4.26 | 5.62 | 6.31 | 0.013 | 0.015 | 0.029 | 0.038 | 0.069 |
| 300G30S2H4 | 3.71 | 5.01 | 5.89 | 0.028 | 0.037 | 0.043 | 0.045 | 0.077 |
| 300G30S2H6 | 3.21 | 4.25 | 5.04 | 0.032 | 0.053 | 0.064 | 0.071 | 0.086 |
| 300G30S4H2 | 3.51 | 4.74 | 4.89 | 0.062 | 0.095 | 0.104 | 0.103 | 0.140 |
| 300G30S4H4 | 3.27 | 4.45 | 4.67 | 0.037 | 0.073 | 0.085 | 0.089 | 0.106 |
| 300G30S4H6 | 2.69 | 3.68 | 4.11 | 0.039 | 0.048 | 0.060 | 0.086 | 0.107 |
| 300G30S6H2 | 3.25 | 4.17 | 5.03 | 0.025 | 0.062 | 0.084 | 0.122 | 0.145 |
| 300G30S6H4 | 3.63 | 4.37 | 4.78 | 0.050 | 0.060 | 0.080 | 0.093 | 0.099 |

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