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1 **Using machine learning techniques for predicting autogenous**
2 **shrinkage of concrete incorporating superabsorbent polymers and**
3 **supplementary cementitious materials**

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10 **Highlights**

- 11 • Experimental data about the influence of SAP on shrinkage were collected
- 12 • Machine learning models predict shrinkage/expansion of concrete with SAP and SCM
- 13 • XGBoost is the most precise machine learning model for shrinkage prediction
- 14 • SHAP and partial difference plots quantify inputs' influence on model results

15

16 **Abstract**

17 Superabsorbent polymers (SAP) are a very effective means of decreasing high-performance
18 and ultra-high performance concrete autogenous shrinkage. However, their efficiency can hardly
19 be predictable because of various parameters: SAP properties, supplementary cementitious
20 materials (SCM) nature, and cement replacement ratios. This study provides a machine learning
21 approach for predicting shrinkage/expansion in cementitious materials incorporating SAP and
22 SCM. A dedicated database is built, and four machine learning models are compared. Extreme
23 Gradient Boosting (XGBoost) model exhibited the highest accuracy. SHapley Additive
24 exPlanations (SHAP) allowed the identification of the most influential inputs, and partial
25 dependence plots provided quantitative information about their relative influence.

26

27 **Keywords:** Concrete; shrinkage; Superabsorbent polymer (SAP); Machine Learning; Gradient Boosting.

28

29 **1. Introduction**

30 Concrete is the most consumed human-made material on Earth due to its cost, strength, and
31 local availability of its components. A wide range of cementitious materials has been developed:
32 from lightweight concrete to self-compacting concrete and high-performance or ultra-high
33 performance concrete. These materials, carefully selected depending on the required mechanical
34 properties and necessary durability depending on their prospective environmental exposure, can
35 be subjected to several types of degradation, one of the most prejudicial being cracking. Cracking
36 can appear due to several reasons during the lifetime of a structure. One of the major causes of
37 cracking during the first weeks after casting is restrained shrinkage which appears when a
38 structural element tends to shrink but cannot shrink due to surrounding elements [1–3].

39 Several shrinkage mechanisms generally add up and produce total shrinkage: chemical
40 shrinkage, plastic shrinkage, autogenous shrinkage, drying shrinkage, thermal shrinkage, and
41 carbonation shrinkage. Within the first days after casting, autogenous shrinkage has been reported
42 as the major shrinkage mechanism in high-strength concrete (HPC) and ultra-high performance
43 concrete (UHPC). These cementitious materials, known for their good mechanical properties and
44 durability, are formulated with limited or small water-to-cement ratios (w/c), generally below 0.4
45 for HPC and 0.3 for UHPC. Self-desiccation develops quickly within the capillary pores as relative
46 humidity drops, creating capillary depressions within the skeleton because of the small amount of
47 water available for cement hydration. Due to these microscopic evolutions, autogenous shrinkage,
48 defined as the external macroscopic volume reduction that occurs under isothermal/sealed
49 conditions, is measured, and cracking might occur within the first days/weeks [4,5].

50 The initial concrete composition greatly influences autogenous shrinkage, and the actual
51 development of cementitious materials, incorporating vast amounts of supplementary cementitious
52 materials, motivates a deep understanding of their relative role in shrinkage [6,7]. First, besides
53 the water-to-cement or water-to-binder (w/b) ratios, it was found that cement fineness generates
54 more autogenous shrinkage, while the higher the aggregate-to-binder ratio, the smaller the
55 autogenous shrinkage due to the restraining effect of aggregates [8]. Then, during the last decades,
56 it was found that autogenous shrinkage is significantly increased by the presence of silica fume in
57 HPC and UHPC, leading to careful monitoring of autogenous shrinkage in such mixes [9,10]. The
58 addition of 5% or 10% silica fume was found to increase significantly autogenous shrinkage, and
59 three main mechanisms are generally used to explain this increase: i) the refined pore structure, ii)

60 the increased formation of CSH with a porous structure due to portlandite consumption and iii) the
61 acceleration of hydration and water adsorption around silica fume particles [6]. To a smaller extent,
62 though this question is still under debate, slag was also found to negatively influence shrinkage in
63 some cases with 30%-50% replacement ratios [11,12], while it was found to create a relative
64 expansion in other studies and specifically in some UHPC mixes. The negative influence of slag
65 on autogenous shrinkage has been related to the increased chemical shrinkage due to slag, chemical
66 shrinkage being a driving force of autogenous shrinkage. At the opposite, fly ash was found to
67 reduce shrinkage for replacement ratios between 15% and 60% because of the slower hydration
68 reaction of mixes incorporating fly ash, but its effect might be limited for smaller replacement
69 ratios [13,14]. Similarly, calcined clay was found to decrease autogenous shrinkage during the first
70 weeks but can increase long-term autogenous shrinkage [15–17], and filler is generally reported to
71 decrease shrinkage, acting as a small aggregate mitigating the shrinkage of the cement paste
72 [18,19]. Due to these adverse effects, the global autogenous shrinkage behavior of complex
73 concrete formulations is worth being investigated, especially in the case of slag and limestone filler
74 blends [20], limestone calcined clay cement (LC3) [21], or eco-friendly ultra-high performance
75 concrete [22,23].

76 Autogenous shrinkage can be mitigated using specific additives in concrete. Several additives
77 have been employed, from natural components to engineered materials [24,25]. First, it was found
78 that some lightweight aggregates can reduce shrinkage due to their intrinsic porosity leading to the
79 gradual release of water during the first days after casting. For example, pumice has been reported
80 to reduce shrinkage considerably [26]. Novel materials have been designed to mitigate shrinkage
81 and subsequent cracking during the last decades. Superabsorbent polymers, which are polymer
82 particles able to store extra water during mixing and restore their water during the first days [27],
83 have also been successfully employed to mitigate concrete shrinkage [28–31] and are further being
84 developed for some years in order to optimize their water absorption capacity and release rate in
85 the high pH concrete matrix. When incorporated in the concrete mix by around 0.2 to 0.6% of
86 cement mass, SAP have been proved to be an effective solution in mitigating autogenous
87 shrinkage, drying shrinkage [32], and stress development [33], although some later deformations
88 might be observed when SAP become empty. The efficiency of SAP, which intrinsically relies on
89 their nature the initial cross-linking and the nature of the chemical components [34], can be
90 assessed before concrete mixing by performing absorption tests on the SAP such as the ‘tea bag
91 method’ and the ‘filtration method’ [35–37]. Though precise chemical information about SAP

92 composition had not been reported systematically [31], SAP with various initial composition and
93 absorption characteristics (either ‘releasing’ or ‘retentive’) have been found effective in reducing
94 autogenous shrinkage [38]. SAP diameter, which was initially assumed to play a role in the
95 shrinkage mitigation capacity, is a less important parameter as long as SAP particles are evenly
96 distributed within the cementitious matrix [39]. Besides their interest concerning autogenous
97 shrinkage mitigation, SAP are also helpful in drying and plastic shrinkage mitigation, enhancing
98 self-healing, and increasing freeze-thaw resistance [31].

99 For the reasons above, a precise understanding of the effect of SAP on the autogenous
100 shrinkage of high-performance and ultra-high performance concrete mixes incorporating
101 supplementary cementitious materials is necessary to anticipate the harmful consequences of
102 cracking in modern concrete. Machine learning predictions would help design such complex
103 materials. Indeed, artificial intelligence techniques have been successfully applied to several Civil
104 Engineering problems such as concrete strength prediction [40,41], creep prediction [42–44], crack
105 assessment in structures [45] or durability and microstructural properties such as surface chloride
106 concentration [46] and and mechanical properties of stabilized soil [47,48]. Among the various
107 techniques developed, ensemble machine learning algorithms applied to datasets with hundreds of
108 data points have proved a good accuracy and robustness against overfitting risk, often associated
109 to conventional techniques and neural networks. Some machine learning models were successfully
110 applied to autogenous or drying shrinkage modeling, but most of them [42,49–51] did not consider
111 SCM, and, to date, no model has been proposed for the shrinkage or swelling prediction of
112 cementitious materials incorporating SAP.

113 This study provides an insight into the potential of machine learning models, based on
114 conventional or ensemble techniques, to predict the autogenous shrinkage / swelling properties of
115 cementitious materials, incorporating supplementary cementitious materials. A database has been
116 specifically built based on the NU database and the available literature. The theory and procedure
117 associated with the models are briefly presented in the manuscript. Then, the results of the models
118 are discussed, and the best model candidate is further examined using SHapley Additive
119 exPlanation (SHAP) theory to understand the most influential features. Finally, partial difference
120 plots are used to quantitatively assess the influence of the features on the shrinkage / swelling
121 predictions.

122 **2. Database description and analysis**

123 Observations of autogenous shrinkage were selected from NU database [52] (187
124 observations) and published studies about autogenous shrinkage of low water-to-cement ratio
125 cement paste, mortar or concrete samples incorporating SCM [5,8,10,11,13–15,17,20,21,53–
126 68,68–74] and / or SAP [28,29,33,39,75–87] (142 and 108 values respectively). In total, 437
127 autogenous shrinkage curves were used to interpolate shrinkage (or swelling) at various ages, e.g.,
128 1d, 2d, 7d, 14d, and 28d. Based on these interpolations, 1889 shrinkage data points were generated,
129 ranging between 1166 $\mu\epsilon$ (swelling with SAP) and -3818.9 $\mu\epsilon$ (shrinkage of a low w/c cement
130 paste). Fourteen parameters have been selected as model inputs: water-cement ratio, water-binder
131 ratio, aggregate-cement ratio, cement content (kg/m^3), silica fume content (% cement mass), fly
132 ash content (% cement mass), slag content (% cement mass), calcined clay content (% cement
133 mass) (denoted as metakaolin), filler content (kg/m^3), amount of superplasticizer (% cement
134 mass), SAP content (% cement mass), SAP size (μm), SAP water uptake (g / g of SAP in cement
135 slurry) and time since the beginning of shrinkage measurements (days). Compressive strength and
136 Young's modulus were deliberately not used as inputs to build a model using only formulation
137 inputs without any need to perform additional experiments. Shrinkage (or swelling) value at a
138 given age was the targeted value. Moreover, as NU database does not include the shrinkage
139 measurement method (among inductive sensors, laser sensors, hydrostatic scales; forming
140 cuboidal samples in foil, corrugated PP tubes, buoyancy method), the shrinkage measurement
141 methodology was not accounted for in the database.

142 Details about the database composition are given in Table 1. Median values of 0.35 and 0.30
143 were obtained for water-to-binder, and water-to-cement ratios resp., which corresponds to average
144 experimental values reported in autogenous shrinkage studies. A median cement content of around
145 $500 \text{ kg}/\text{m}^3$ was obtained, which is consistent for this type of study. Histograms of the input and
146 output values are given in Fig. 1. As illustrated in Fig. 1 k), SAP contents of 0.2, 0.4, and 0.6 %
147 cement mass were mostly used in the studies selected to build the database.

148 Histograms of the input data are given in Fig. 1. Correlations between the variables were
149 calculated prior to machine learning algorithms application. The correlation matrix is given in Fig.
150 2. As expected, the first four parameters (water-cement ratio, water-binder ratio, aggregate-cement
151 ratio, cement content) were particularly correlated and relatively well correlated with autogenous
152 shrinkage / swelling values. Interestingly, the three variables concerning SAP were found to be
153 correlated too, highlighting common practices when using SAP such as adapting the SAP content

154 depending on SAP swelling capacity [88] and selecting SAP size depending on the application, for
 155 example, autogenous shrinkage reduction, leading to a correlation with SAP swelling capacity.

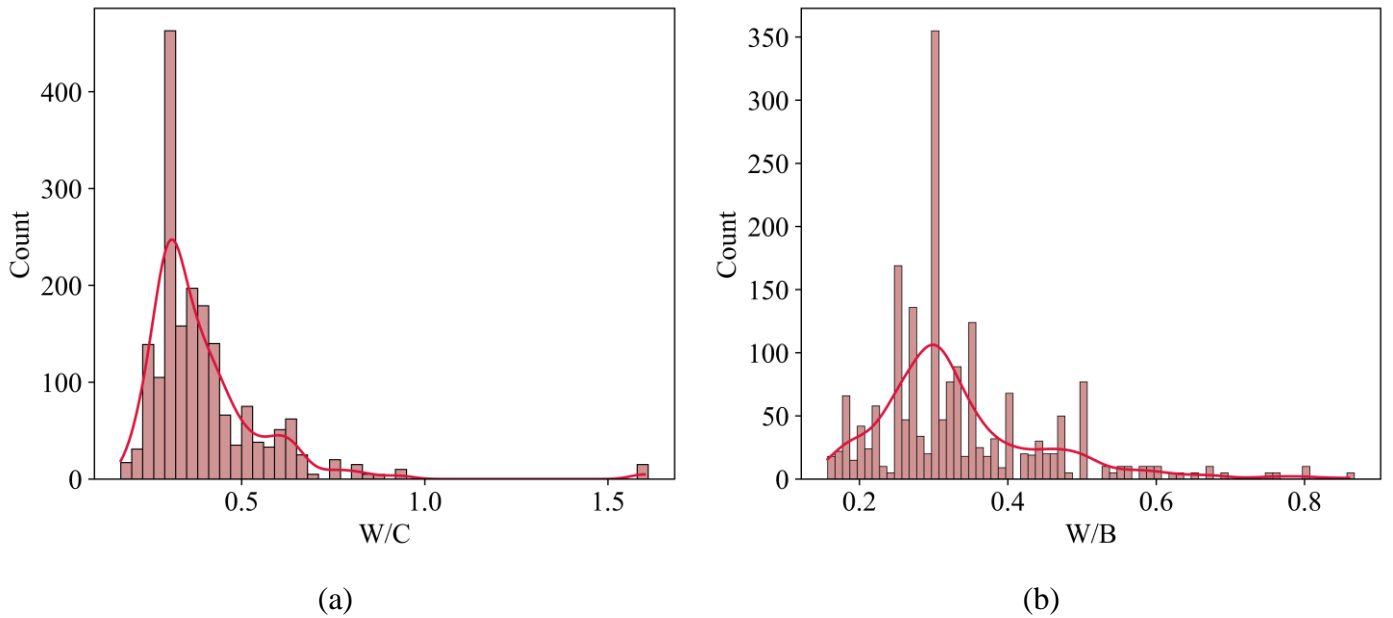
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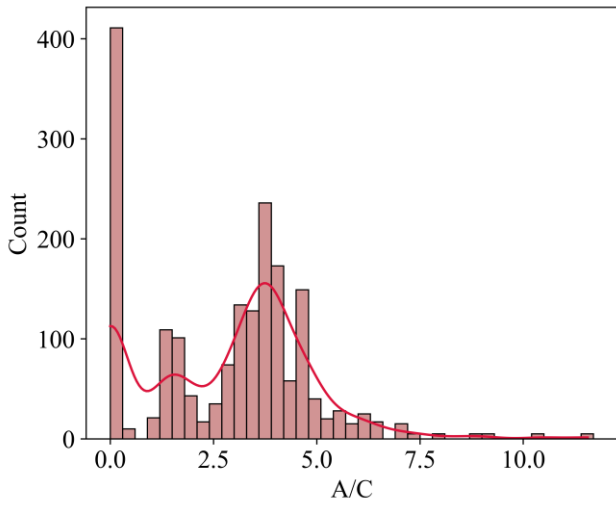
157 **Table 1.** Description of the database used in this study

	No	Unit	Count	Mean	Median	Min	Max	Q _{25%}	Q _{75%}	Std	Skw
W/C	1	-	1889	0.40	0.35	0.17	1.60	0.3	0.44	0.17	3.36
W/B	2	-	1889	0.33	0.3	0.157	0.86	0.266	0.374	0.11	1.49
A/C	3	-	1889	2.83	3.28	0	11.56	1.24	4.02	2.02	0.33
Cement	4	kg/m ³	1889	637.41	498	167.4	1762.00	418	700	364.99	1.53
Silica fume	5	(*)	1889	4.80	0	0	50.00	0	10	8.44	2.32
Fly ash	6	(*)	1889	5.13	0	0	100.00	0	0	14.32	3.21
Slag	7	(*)	1889	8.05	0	0	400.00	0	0	36.71	7.28
Metakaolin	8	(*)	1889	0.70	0	0	57.40	0	0	4.85	9.46
Filler	9	(*)	1889	4.51	0	0	125.00	0	0	13.83	3.98
Superplasticizer	10	(*)	1889	1.39	0.8	0	11.82	0	1.8	1.98	2.49
SAP	11	(*)	1889	0.06	0	0	0.92	0	0	0.16	2.68
SAP size	12	μm	1889	43.01	0	0	645.00	0	0	107.15	3.33
SAP water uptake	13	(**)	1889	4.51	0	0	61.00	0	0	10.89	3.32
Time	14	days	1889	9.06	7	1	28.00	2	14	9.40	1.08
Shrinkage/Swelling		μϵ	1889	-280.93	-136.6	-3818.9	1166.70	-382.2	-26.4	491.77	-2.69

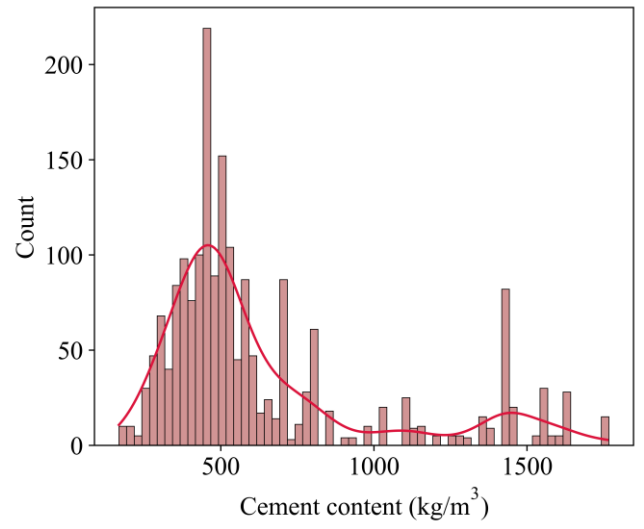
158 (*) % cement mass; (**) g/g of SAP; Skw=Skewness; Std=Standard deviation;

159

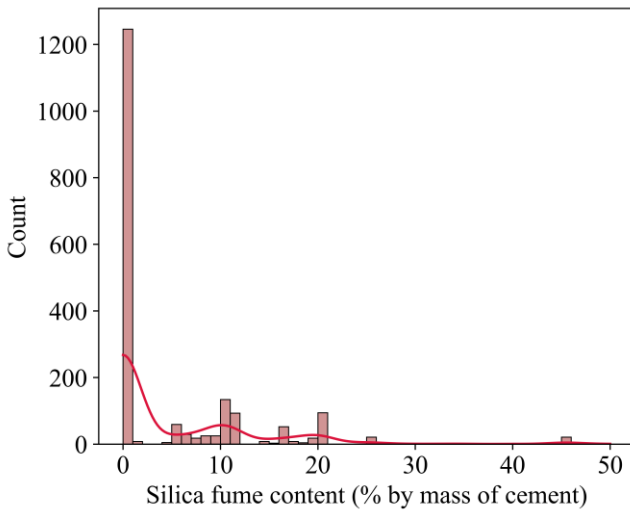




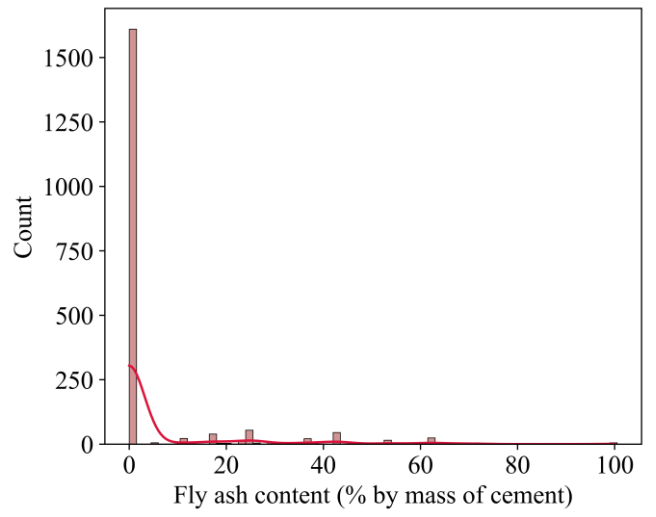
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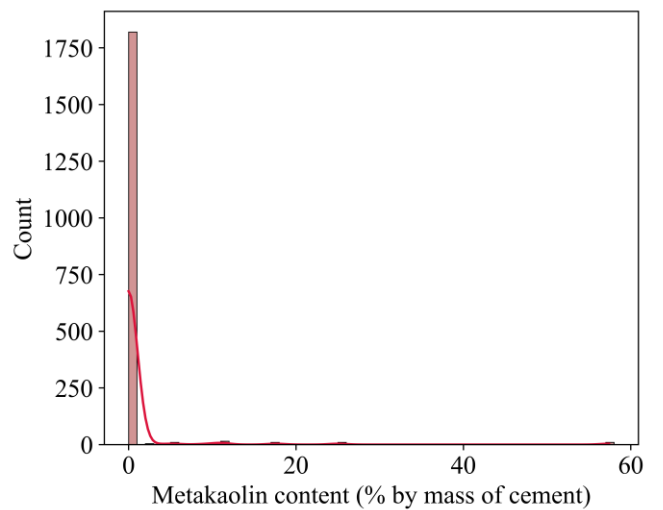
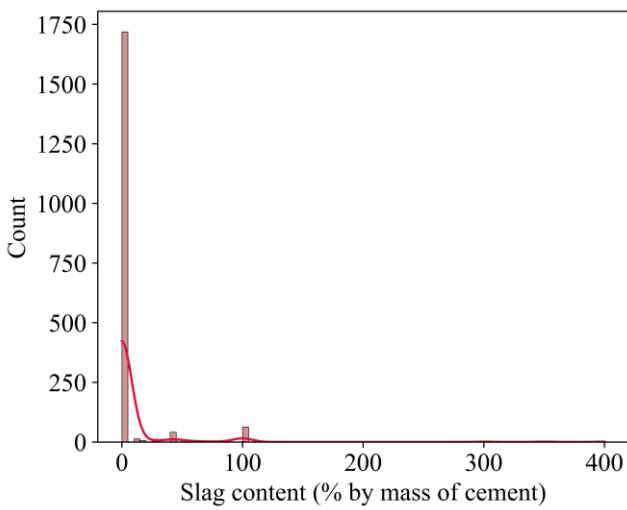
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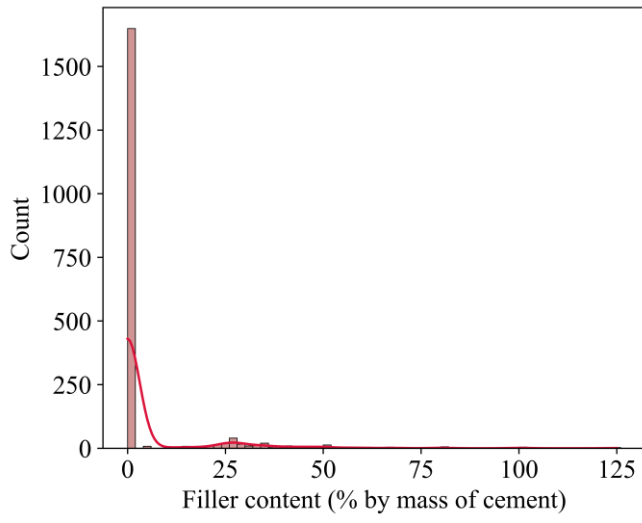
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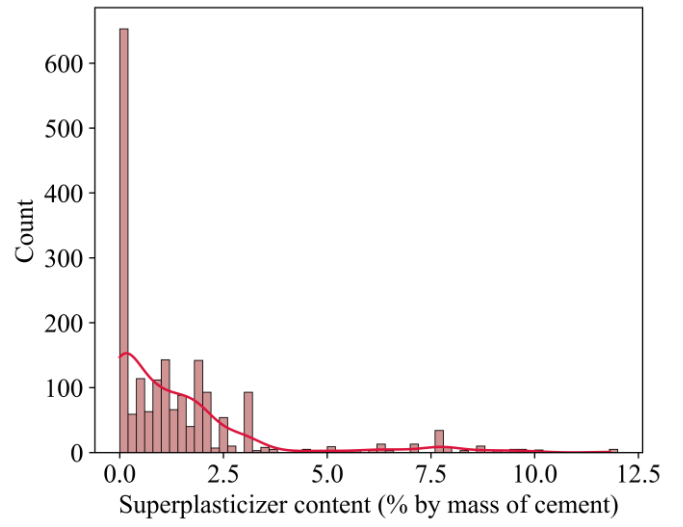
(f)



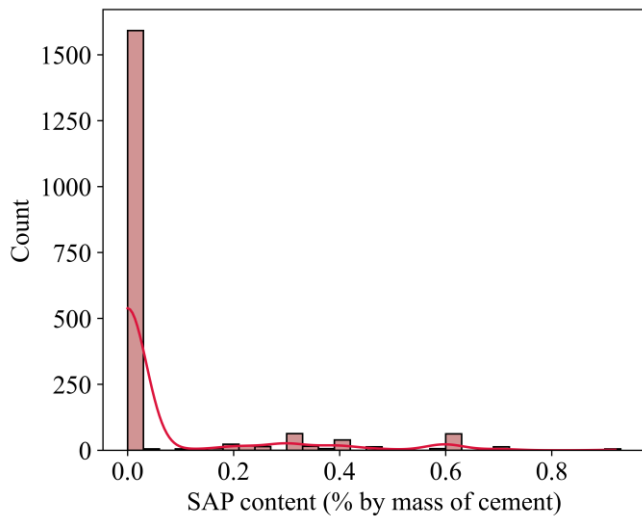
(g)



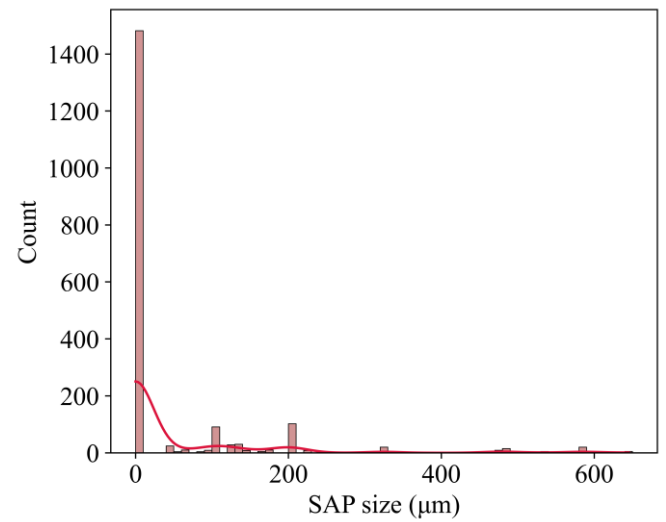
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(i)

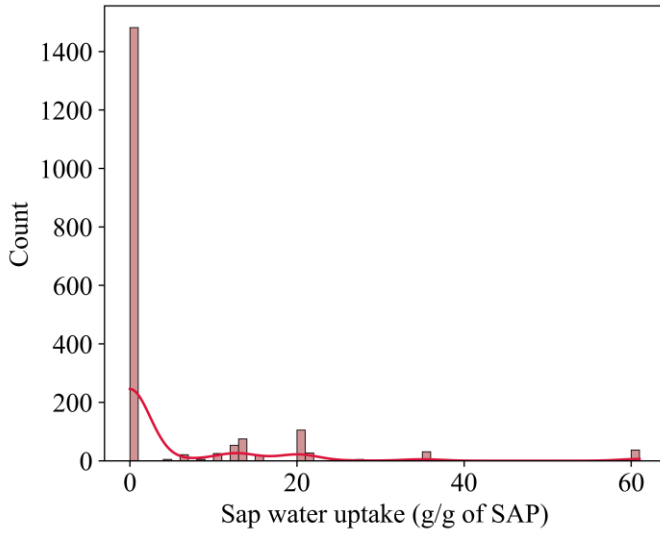


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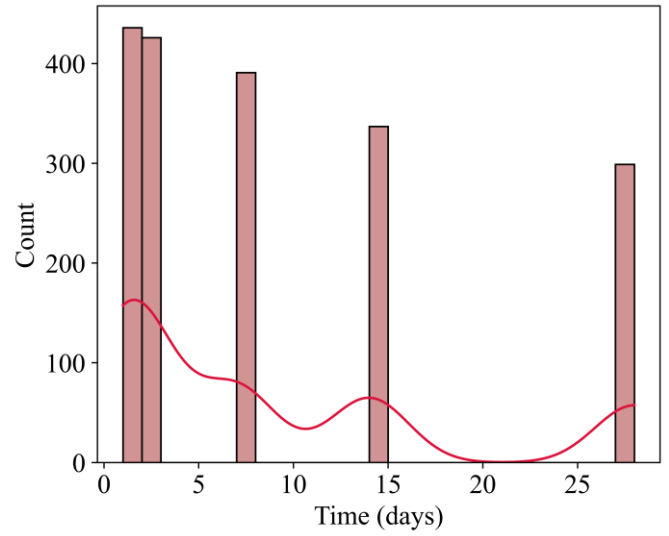


(k)

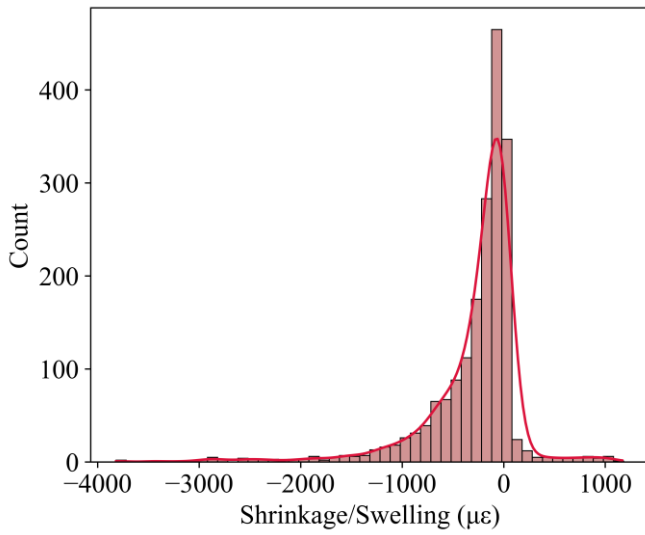




(m)



(n)



(o)

160 **Fig. 1.** Data distribution of each input variable and the output variable (shrinkage/swelling).

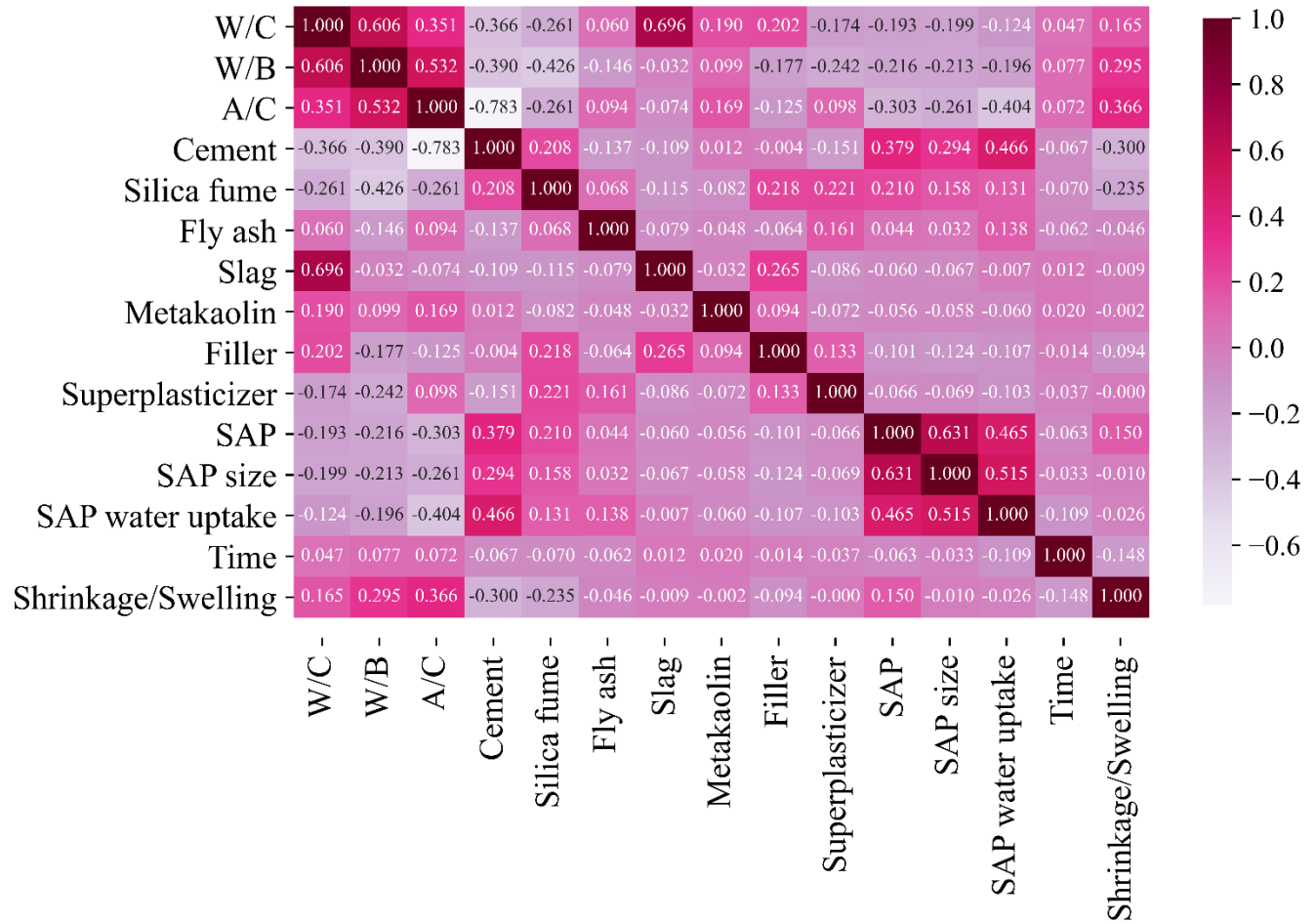


Fig. 2. Correlation matrix of the input and output variables

3. Machine Learning Methods

In this study, four kinds of state-of-the-art Machine Learning (ML) models have been used, three of them being ensemble models, generally the best models for medium tabular data encountered in Civil Engineering problems. The four ML algorithms: K-Nearest Neighbors (KNN), Random Forest (RF), Gradient Boosting (GB), and Extreme Gradient Boosting (XGB), are briefly presented in this section. As the performances of ML models depend strongly on their hyperparameters, the default hyperparameters used in Sklearn were selected, which helps reduce the time of building ML model. The Monte Carlo simulation (MCS) is chosen as a validation technique for evaluating the performance of ML models. The MCS and k-fold cross-validation are two common validation techniques. However, the MCS can give the results with higher confidence and lower variance than the k-fold cross-validation technique.

3.1. K-Nearest Neighbors (KNN)

175 The k-nearest neighbors' algorithm (k-NN) is a non-parametric classification method invented in
176 1951 by Fix and Hodges [90] and later extended by Altman [91]. The input in both cases consists
177 of the k closest training examples in a data collection. The result of k-NN regression is the object's
178 property value. This value is the mean of the values of the k closest neighbors. A good strategy is
179 to apply weights to the contributions of the neighbors, such that closer neighbors contribute more
180 to the average than the neighbors who are farther away. Neighbors-based regression is a sort of lazy
181 learning in that it does not seek to build a generic internal model and instead just saves instances of
182 the training data [92]. As an average or local linear approximation, the regression result is obtained
183 from the k-nearest neighbors of each point. This technique is easy to construct, resistant to noisy
184 training data, and effective with huge amounts of training data. However, the value of k must be
185 determined, and the calculation cost is high since it must compute the distance of each instance to
186 all of the training examples.

187 **3.2. Random Forest (RF)**

188 Random forest (RF) is an ensemble learning technique used for classification, regression, and other
189 applications. The RF method incorporates two powerful ML approaches, bootstrap aggregation [93]
190 and random subspace [94]. Bagging generates n bootstrap sets by sampling with replacement N
191 training instances from the training set. The number of bootstrap samples and features is arbitrary
192 and is fewer than the original training set. Then, as illustrated in Fig. 3, each bootstrap set is
193 generated as a decision tree (e). A decision tree identifies a bootstrap set by examining its properties
194 at each node. Each node checks a specific property, with the tree's leaves reflecting the result labels.
195 Moving down a certain tree branch evaluates specific properties at each node to arrive at an output
196 label. The final result combines the outputs of all leaves [95]. The RF prediction output may be
197 written as follows:

$$Y = \frac{1}{n_{trees}} \sum_{i=1}^{n_{trees}} Y_i(x) \quad (1)$$

198 Where Y is the average output of a total number of n_{trees} ; $Y_i(x)$ the single prediction of a tree for an
199 input vector x .

200

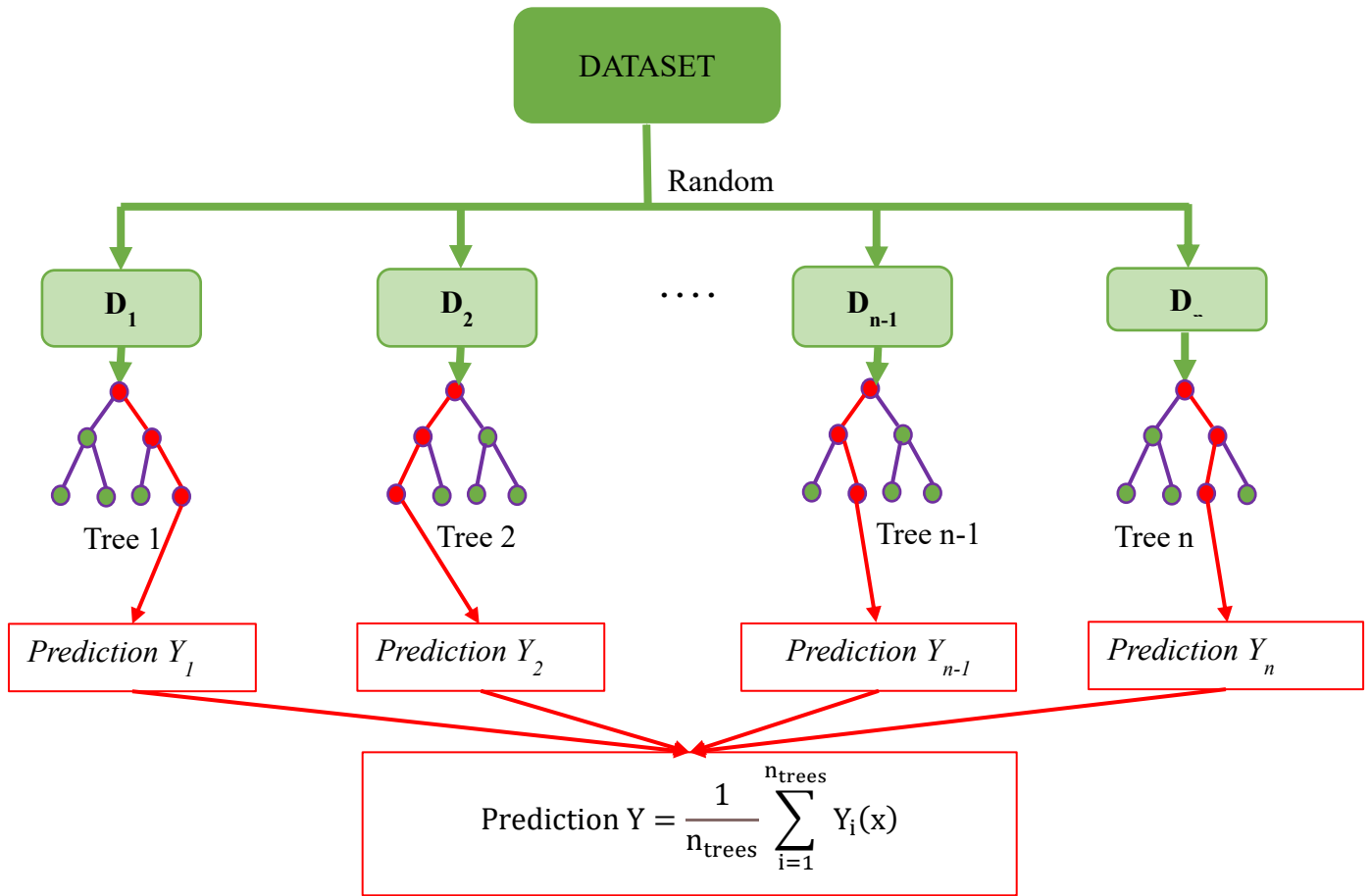


Fig 3. Schematic view of Random Forest

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203

204 **3.3. Gradient Boosting (GB)**

205 Gradient boosting algorithm (GB), like random forest, is an ensemble approach that belongs to a
 206 family of techniques that use many classifications or regression trees in its algorithm to provide a
 207 reliable and desired output. In GB, classification or regression trees, also known as base learners,
 208 are built consecutively to increase the algorithm's performance. GB was originally designed for
 209 classification problems exclusively, though Friedman expanded it to regression challenges [96].
 210 During each iteration, the GB algorithm considers the previously ensemble tree mistake and
 211 attempts to recover the error while predicting the next tree. As a result, the inaccuracy in future
 212 tree ensembles is constantly decreasing. Furthermore, GBM is based on the notion of boosting, in
 213 which numerous combinations of models with high bias and low variance are used to substantially
 214 reduce the high bias while preserving the low variance. This means that GBM combines numerous
 215 shallow trees to increase prediction performance. The shallow trees are learned using the same
 216 dataset as the deep trees. It is worth noting that the gain in prediction performance has endeared it

217 to many academics from other fields, including civil engineering [97,98].

218 **3.4. Extreme Gradient Boosting (XGB)**

219 The XGB model is a sophisticated tree boosting method [99]. It is an enhancement to Friedman's
220 gradient boosting approach [96]. It predicts the outcome using a number of additive functions.

$$\bar{Y}_i^k = \bar{Y}_i^{(k-1)} + \alpha f_k \quad (2)$$

221 where \bar{Y}_i is the predicted result for the i_{th} sample, and x_i is the vector of features; N is the number
222 of estimators, and each estimator f_k (with k ranging from 1 to N) corresponds to an independent
223 tree structure; Y_i^0 is the initial guess, which is the mean of the measured values in the training set;
224 and α is the learning rate which helps to improve the model smoothly while adding new trees and
225 avoid overfitting It is worth noting that overfitting is the primary problem with all ML models.
226 The training procedure is carried out in an additive manner. According to Eq. 2, at the k_{th} step, a
227 k_{th} estimator is added to the model, and the k_{th} expected result \bar{Y}_i^k is determined by subtracting
228 the predicted value at the previous stage $\bar{Y}_i^{(k-1)}$ from the estimation f_k of the extra k_{th} estimator. f_k
229 is determined by the leaf weights discovered by minimizing the objective function of the k_{th} tree
230 specified by:

$$objective = \lambda T + \sum_{j=1}^T \left[E_j \omega + \frac{1}{2} (F_j + \gamma) \omega_j^2 \right] \quad (3)$$

231 where T is the number of k_{th} tree leaves and x_j with j ranging from 1 to T are the leaf weights; λ
232 and γ are regularization parameters that govern the tree structure's simplicity to minimize
233 overfitting. The parameters E_j and F_j , which are the sums of the samples associated with the j_{th}
234 leaf of the loss function's first and second gradients, respectively.

235 Starting with a single leaf, the k_{th} tree is built by separating the leaves. This technique is carried
236 out by maximizing the gain parameter, which is described by:

$$gain = \frac{1}{2} \left[\frac{E_L^2}{F_L + \gamma} + \frac{E_R^2}{F_R + \gamma} - \frac{(E_L + E_R)^2}{F_L + F_R + \gamma} \right] - \lambda \quad (4)$$

237 After the splitting, E_L and F_L are linked with the left leaf, while E_R and F_R are associated with

238 the right leaf. If the gain parameter is greater than zero, the splitting is accepted. As a result, raising
 239 the regularization parameters λ and γ reduces the gain parameter, allowing the tree structure to
 240 remain simple by avoiding the complexity of leaf splitting. However, it will impair the model's
 241 ability to fit the training data.

242 3.5. Performance evaluation of models

243 The model performances were evaluated using the following three metric indexes: coefficient
 244 of determination (R^2), root mean square error (RMSE) and mean absolute error (MAE), whose
 245 formulations are given as follows:

$$R^2 = \frac{\sum_{j=1}^N (p_{0,j} - \bar{p}_0)(p_{t,j} - \bar{p}_t)}{\sqrt{\sum_{j=1}^N (p_{0,j} - \bar{p}_0)^2 \sum_{j=1}^N (p_{t,j} - \bar{p}_t)^2}} \quad (5)$$

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{j=1}^N (p_{0,j} - p_{t,j})^2} \quad (6)$$

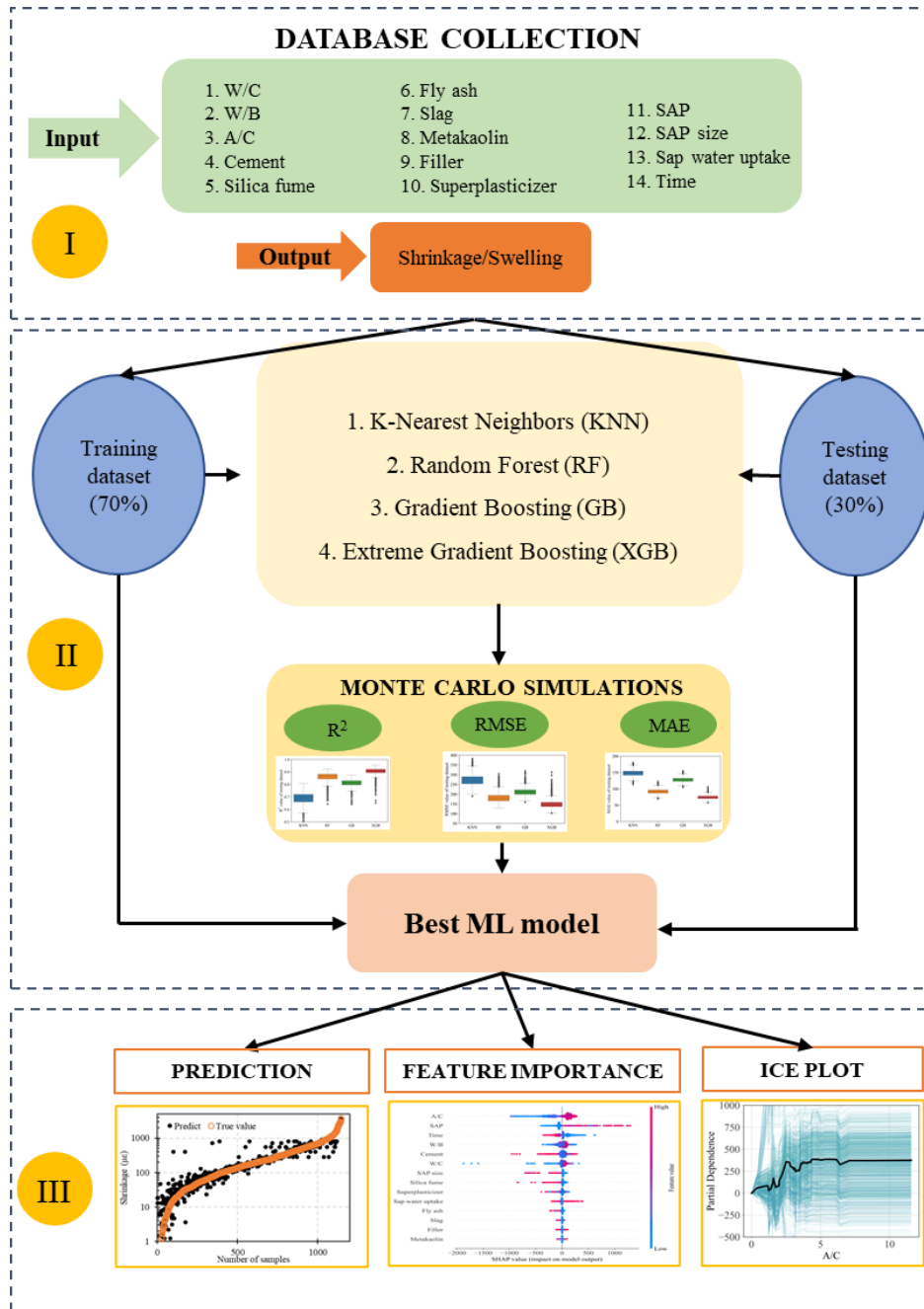
$$\text{MAE} = \frac{1}{N} \sum_{j=1}^N |p_{0,j} - p_{t,j}| \quad (7)$$

246 Where $p_{0,j}$ is the shrinkage/expansion value of i-th sample point in the database; $p_{t,j}$ is the
 247 prediction value made by machine learning models for i-th sample point; \bar{p}_0 is the averaged
 248 experimental value of shrinkage / expansion and \bar{p}_t is the mean predicted value. Both MAE and
 249 RMSE explicitly characterize the residual error at each sample point and can give an exact
 250 evaluation of the model performance. In comparison, R^2 normalizes the squared residual error with
 251 the variance of the database and produces dimensionless scores ranging from 0 to 1. Because
 252 RMSE is generally considered more intuitive as it is comparable to measured values and
 253 convenient for comparing the performance of different models, it has been adopted as the main
 254 metric index in the following analysis

255 3.6. Methodology flow chart

256 The methodology diagram reported in Fig. 4 displays the investigation's design. The concept is
 257 separated into three key steps: step (I) database preparation and description, step (II) selection of
 258 the best ML model with the highest performance, and step (III) Shrinkage/Swelling prediction and

259 sensitivity analysis. In step one, samples are collected from various literature studies, including input
260 and output variables. The database used to predict the shrinkage/swelling of concrete has fourteen
261 input variables: W/C, W/B, A/C, Cement content, Silica fume content, Fly ash content, Slag content,
262 Metakaolin content, Filler content, Superplasticizer content, SAP content, SAP size, SAP water
263 uptake and time. In step two, the database is randomly divided into 70% for training (1322 samples)
264 and 30% for testing (567 samples). Four ML models comprised of algorithms such as KNN, RF,
265 GB, and XGB are employed for training the ML model. The coefficient of determination R^2 , Root
266 Mean Square Error RMSE, and Mean Absolute Error MAE are used to evaluate ML performance.
267 The Monte Carlo Simulation MCS is used to analyze the performance of four ML models in order
268 to select the best ML model using the default hyperparameters. In the final step, the best ML model
269 is used to predict the shrinkage/swelling of concrete and assess the effect of each factor on the
270 shrinkage/swelling of concrete using Shapley Additive Explanations (SHAP) and partial
271 dependency analysis, including Individual Conditional Expectation Plots (ICE) [100].



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273
274

Fig 4. Conception of shrinkage/swelling investigation

275 **4. Results and Discussion**

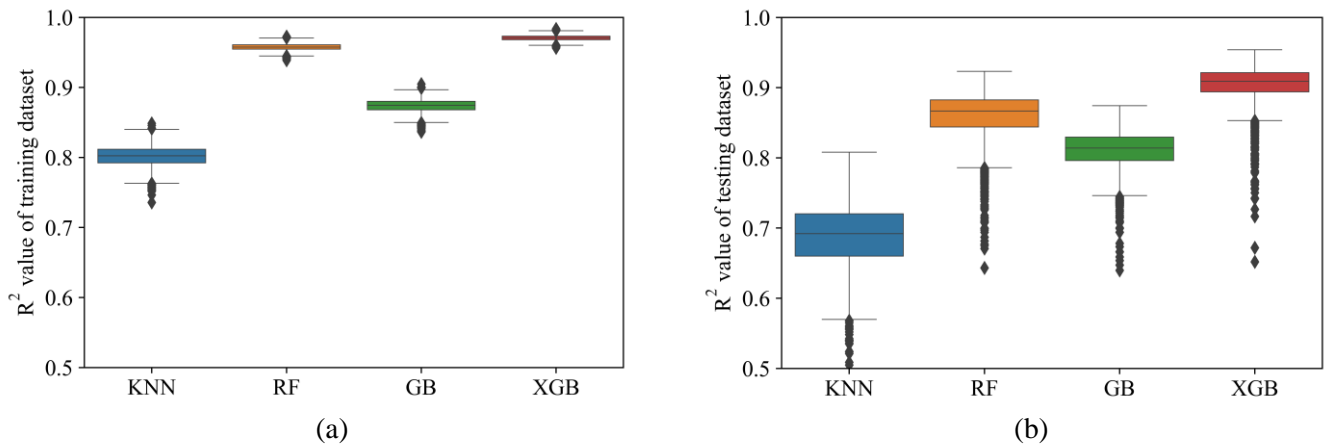
276 **4.1. Performance evaluation of machine learning models**

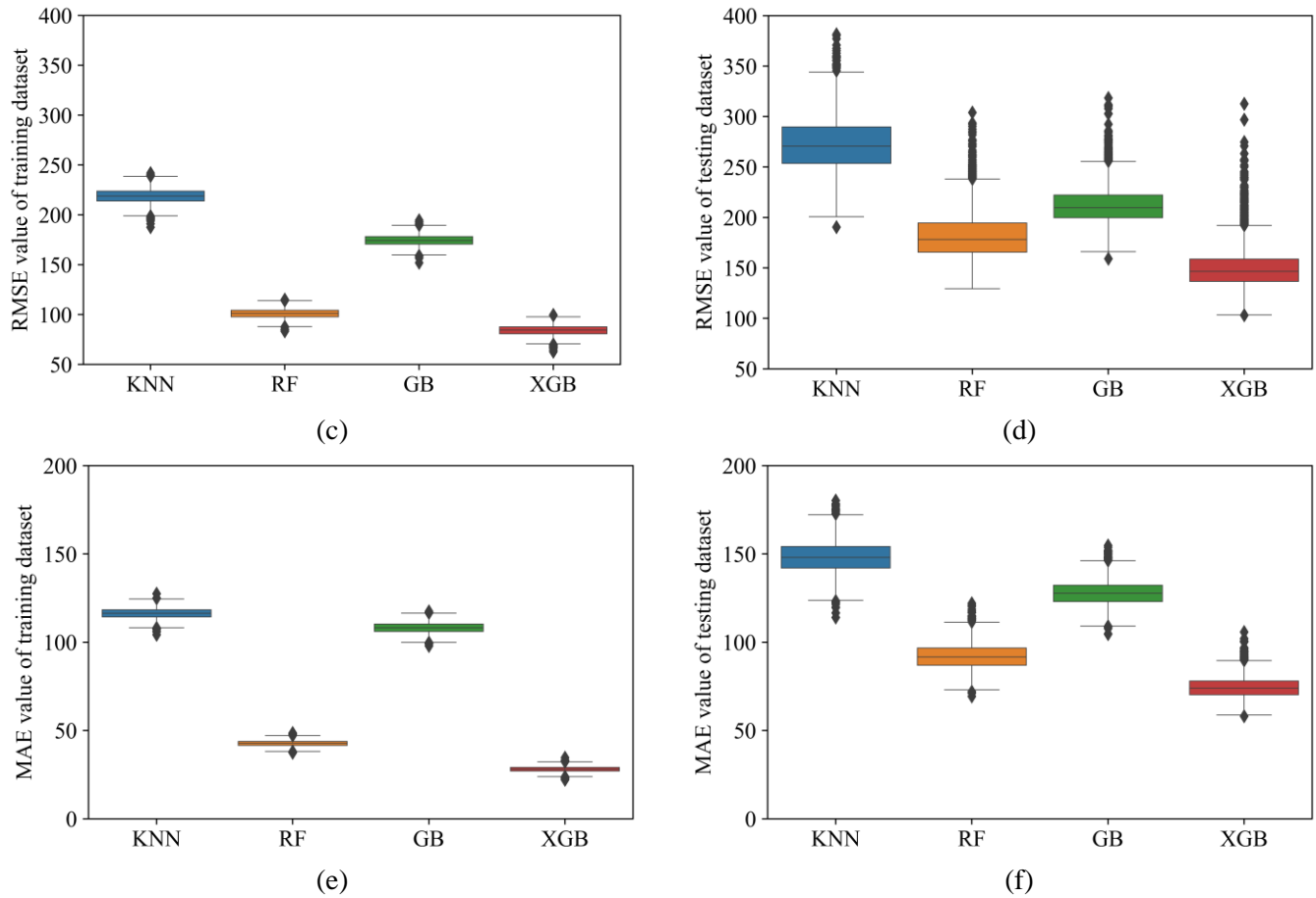
277 The performance of the four models on the testing set has been evaluated using the metrics
278 mentioned above for 3000 simulations varying the initial train-test split. Random Forest and
279 XGBoost algorithms performed significantly better than Gradient Boosting and K-Nearest

280 Neighbors on the training and testing sets, as illustrated in Fig.5.

281 The generalization capacity of the models has been evaluated by predicting the shrinkage /
282 swelling values of the 567 samples in the test set. Minor discrepancies were observed between the
283 accuracy of the training set and the testing set. The extent of overfitting was measured as marginal
284 and therefore has been reasonably neglected. As illustrated in Fig. 5, comparing the performance
285 of the four models, RF and XGBoost obtained the best results on the test set during training. The
286 mean values of the performance metrics of the four models have been reported in Table 2. Mean
287 R^2 values of 0.958 and 0.971 were obtained on the training set using RF and XGBoost models
288 resp. These values correspond to small RMSE values of 101 $\mu\epsilon$ and 84 $\mu\epsilon$ resp. Despite the limited
289 data, mean performance metrics were good on the test data. Mean R^2 values of 0.859 and 0.904
290 were obtained on the test set using RF and XGBoost models resp. These values correspond to
291 limited RMSE values of 183 $\mu\epsilon$ and 150 $\mu\epsilon$ resp.

292 The best prediction performance has been obtained using the XGBoost model. With this
293 model, R^2 and RMSE values of 0.954 and 111.6 $\mu\epsilon$ have been obtained. These values are on par
294 with other values reported for autogenous or drying shrinkage predictions reported in the literature
295 [49,50] and calculated RMSE is consistent with the variability of shrinkage measurements
296 obtained during a round Robin test [76].





297
298 **Fig. 5.** Performance of machine learning models after 3000 simulations
299

300 **Table 2.** Comparison of machine learning algorithms for autogenous shrinkage/expansion
301 prediction of concrete incorporating SAP using mean performance value

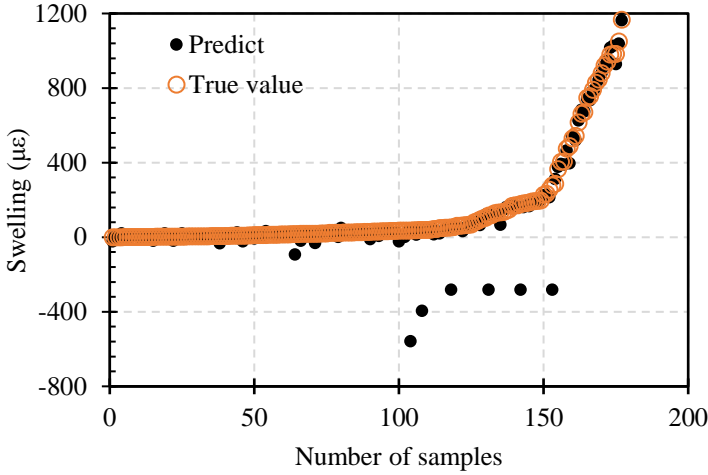
Algorithm	Training set			Test set		
	R ²	RMSE/ $\mu\epsilon$	MAE/ $\mu\epsilon$	R ²	RMSE/ $\mu\epsilon$	MAE/ $\mu\epsilon$
KNN	0.802	218.667	116.332	0.688	272.809	148.203
GB	0.874	174.378	108.200	0.811	212.455	127.898
XGB	0.971	84.103	28.061	0.904	150.337	74.457

302
303 **4.2. Shrinkage/Swelling Prediction of typical machine learning model**

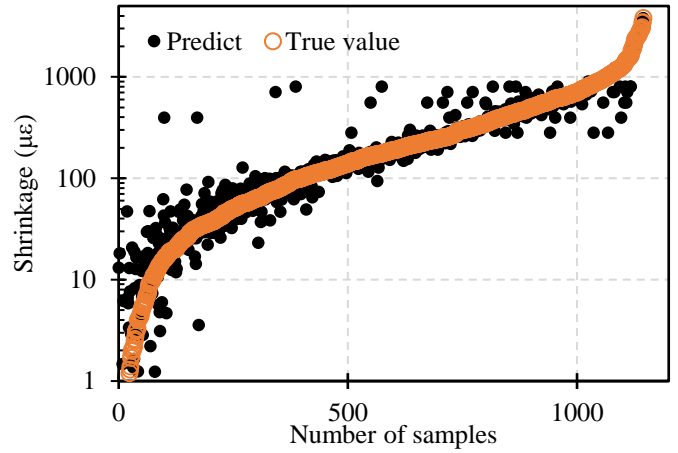
304 The performance of a typical XGBoost model during training and testing is illustrated in Fig.
305 6 and 7. As illustrated in Fig. 6 a) and b), the model performed well on the training dataset for
306 shrinkage and swelling. Only six data points over 175 (around 4 %) were misclassified as

307 shrinkage values while they were relatively small swelling values. As illustrated in Fig 6 b), the
308 model correctly captured the shrinkage phenomenon, and only a few data points were not correctly
309 predicted on the training set. The model predictions, illustrated in Fig. 6 c) and d) agreed with the
310 measured values. As illustrated in Fig. 6 c), the model could correctly predict the swelling values
311 higher than $100 \mu\epsilon$ when SAP were included in the mix for 20 data points, and only relatively
312 limited errors were produced on samples exhibiting swelling values close to $0 \mu\epsilon$. Shrinkage
313 values, represented in Fig. 6 d), were predicted with very good precision for most of the samples
314 in the test set. Only a small portion of predictions was found relatively far from the actual measured
315 values: some shrinkage values were overestimated while actual values were smaller than
316 $50 \mu\epsilon$.(top left part of the figure) while six predictions were clearly underestimated for actual
317 measured values between 50 and $350 \mu\epsilon$.

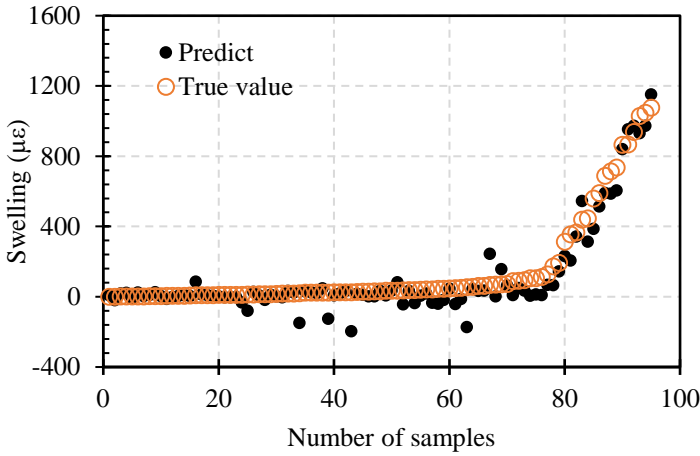
318 The histograms of the errors between predicted and actual values are reported in Fig. 7. The
319 errors were almost symmetric for both the train and the test sets. A small standard error was
320 observed in the case of the training set, and a slightly larger standard error was made on the test
321 set.



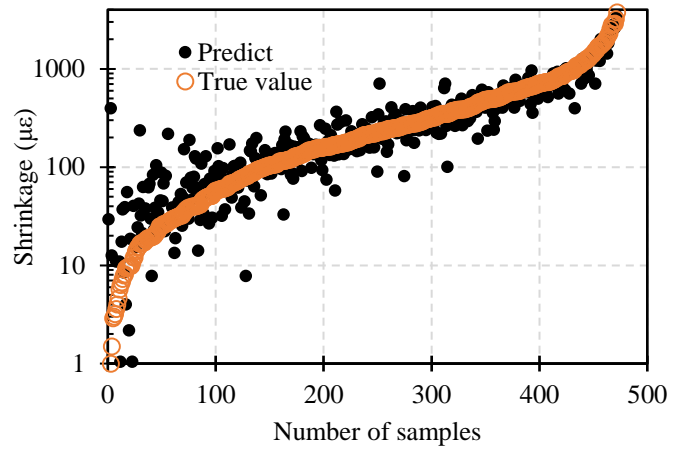
(a)



(b)

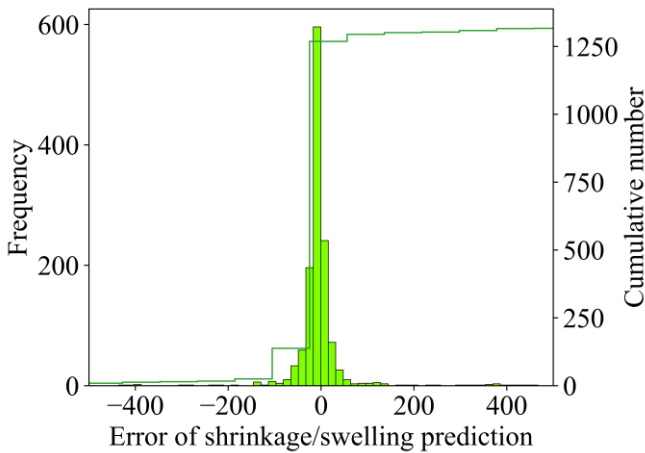


(c)

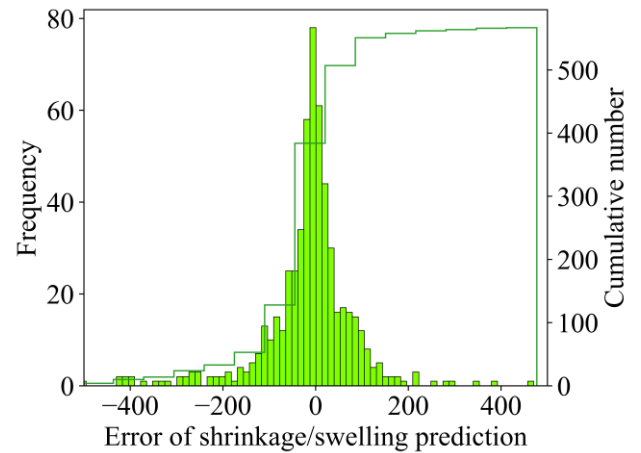


(d)

322 **Fig. 6.** Comparison between target and calculated outputs of typical XGB model for training and
 323 testing database



(a)



(b)

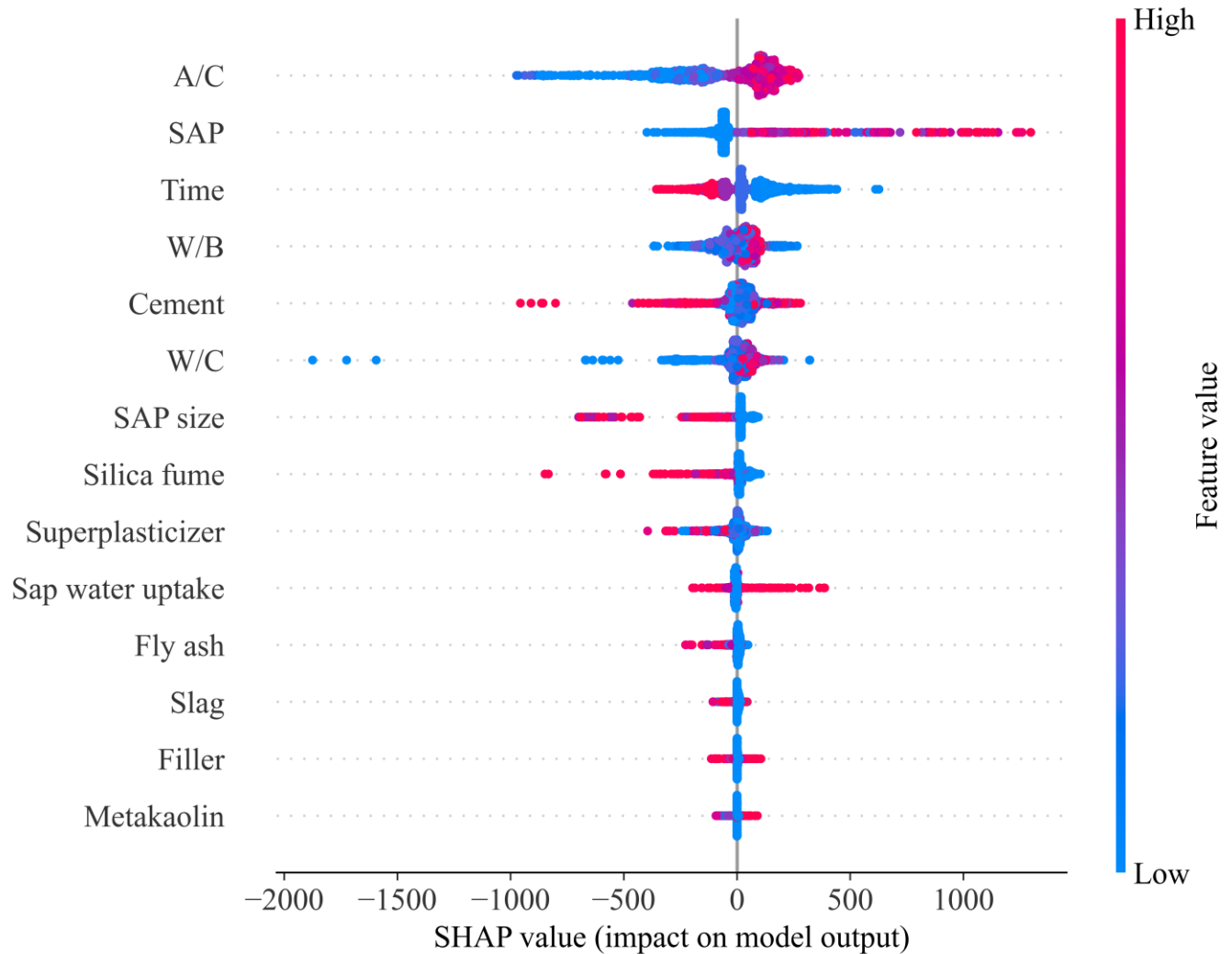
324 **Fig. 7.** Histograms of the error values between predicted and experimental shrinkage/expansion values
 325 for (a) training part, (b) testing part.

326 **4.3. Feature importance analysis using Shapley Additive Explanations (SHAP)**

327 In this study, the SHaple Additive exPlanation (SHAP) provides both local and global
328 interpretations of each input parameter. SHAP provides comparable information to feature
329 importance which has been largely used in the literature, but is more appropriate to ensemble
330 machine learning models as it is more stable and provides quantitative information.

331 The SHAP values of each feature, sorted in order of their average SHAP value, are shown in
332 Fig. 8. The features listed on top of the graphical representation can be associated with the larger
333 contributions to the model outputs. The most influencing parameters on shrinkage predictions were
334 the aggregate-to-cement ratio (A/C), the SAP content, time (days since the beginning of shrinkage
335 measurements), water-to-binder ratio, cement content, water-to-cement ratio, SAP size, and silica
336 fume content. A clear boundary can be observed for all these parameters between high and low
337 feature values influence on the model output: high A/C ratio increases SHAP value, that is to say,
338 decrease shrinkage; high SAP content decreases shrinkage and, most of the time, this was found
339 to be the most influential parameter; high time values correspond to higher shrinkage values; high
340 w/b and w/c tend to decrease shrinkage while high silica fume replacement ratio or cement content
341 mostly induces higher shrinkage, and large SAP size decreases SAP beneficial effect and increases
342 shrinkage compared to smaller SAP sizes. These influences are in agreement with experimental
343 observations.

344 The less influencing parameters were identified: superplasticizer, fly ash, slag, filler, and
345 calcined clay content. These observations based on the SHAP values are consistent with the
346 experimental observations as these parameters are known to have a more negligible influence on
347 shrinkage than the ones mentioned above.



348

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Fig.8. Feature importance analysis using the Shap library in Python code

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4.4. Partial dependence plot analysis for shrinkage/swelling prediction

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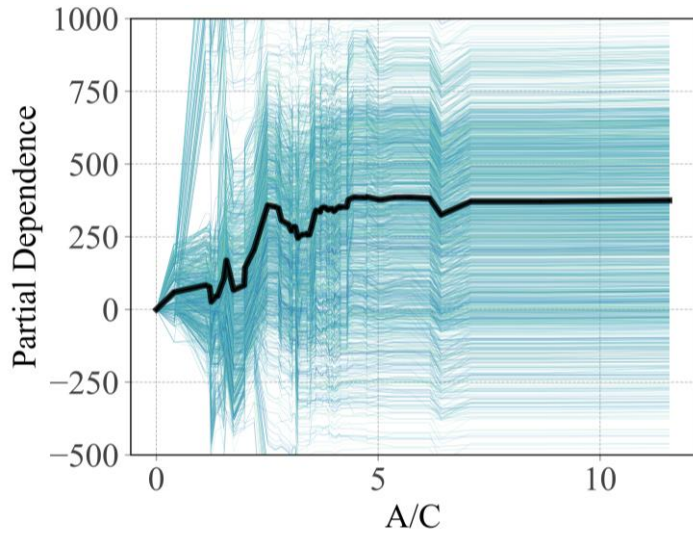
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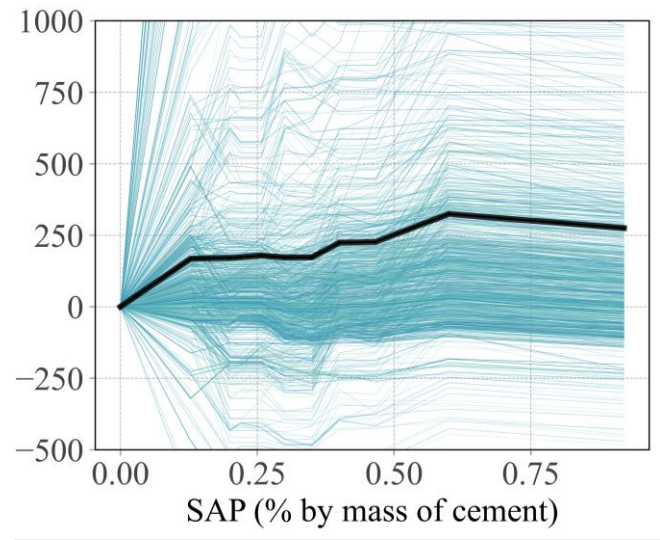
More information about the model predictions can be obtained using the partial difference plots, which represent the quantitative influence of any given parameter on the output. The partial difference plots of each parameter on the output are illustrated in Fig. 9, the most influencing parameters first. As illustrated in Fig 9 a), shrinkage gradually decreases with the increase of the A/C ratio for ratios between 0 and around 5. A mean shrinkage decrease of around $350 \mu\epsilon$ was predicted by the model between A/C ratio of 0 and A/C ratio of 5 which corresponds to the transition from pure cement paste to normal concrete. Also, as illustrated in Fig. 9 b), SAP content also decreases shrinkage almost regularly between SAP content equal to 0 % of the cement mass and around 0.6 % of the cement mass. On average, shrinkage was reduced by around $300 \mu\epsilon$ when

360 an amount of SAP equal to 0.6% of the cement mass was used compared to formulations without
361 SAP. For SAP contents higher than 0.6 % of the cement mass, the model predicted a decrease of
362 the partial dependence, highlighting a limited interest in including more SAP. SAP diameters
363 higher than 100 μm were found to slightly decrease the beneficial impact of SAP as they were
364 associated with partial dependence values around 200 $\mu\epsilon$ smaller than smaller SAP sizes around
365 50-60 μm . No major influence of SAP water uptake could be detected using partial dependence
366 plots, which can be attributed to the fact that the database only included positive published results,
367 i.e., results with beneficial impact of SAP whatever their water uptake.

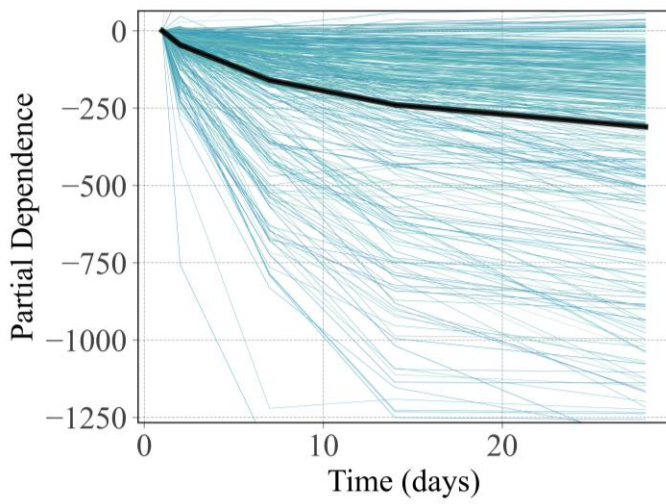
368 As expected, the partial dependence of shrinkage decreased with time, and the global trend is
369 very similar to a shrinkage curve in all the cases (Fig. 9 c)). Water-to-binder and water-to-cement
370 ratios particularly influence autogenous shrinkage for values smaller than 0.4 as illustrated in Fig
371 9 d) and f). On average, shrinkage was predicted 500 $\mu\epsilon$ higher in the case of a water-to-binder
372 ratio of 0.2 compared to a water-to-binder ratio of 0.4. Although the other parameters were not
373 found as important by the model, partial dependence plots show that the model predicted
374 increasing shrinkage values with increasing amounts of silica fume and slag (Fig 9 h), k) and l))
375 as commonly admitted in the literature but predicted an increase of shrinkage with fly ash content
376 which is not in agreement. Contrarily to results reported in the literature, fly ash increased
377 shrinkage on average. However, this result can be attributed to outliers associated with negative
378 partial differences close to -400 $\mu\epsilon$ that particularly influence the results even if most predictions
379 were associated with no effect. Filler and calcined clay showed little influence, which is in
380 relatively good agreement with the literature. The model would benefit from additional literature
381 on these latest points, but studies dissociating the influence of fillers and calcined clay from the
382 other SCM are scarce.



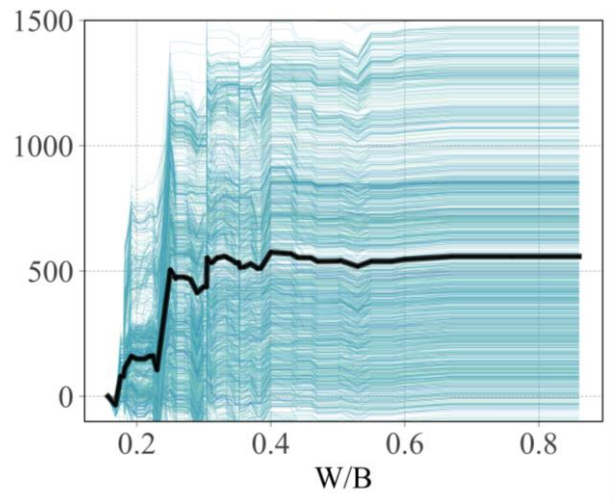
(a)



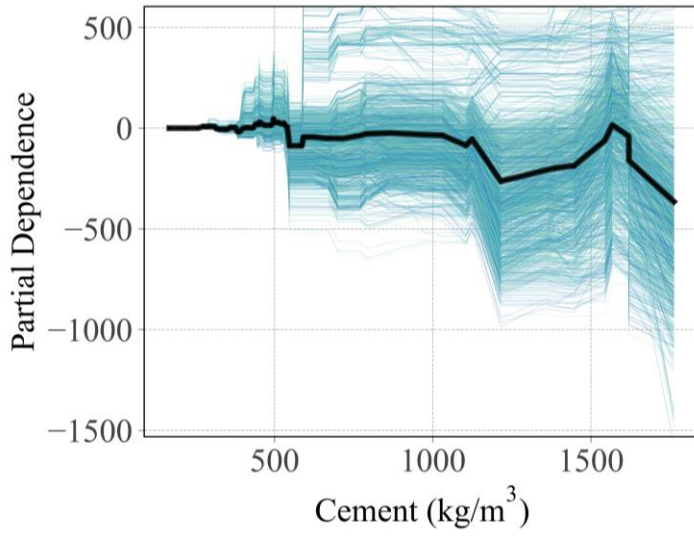
(b)



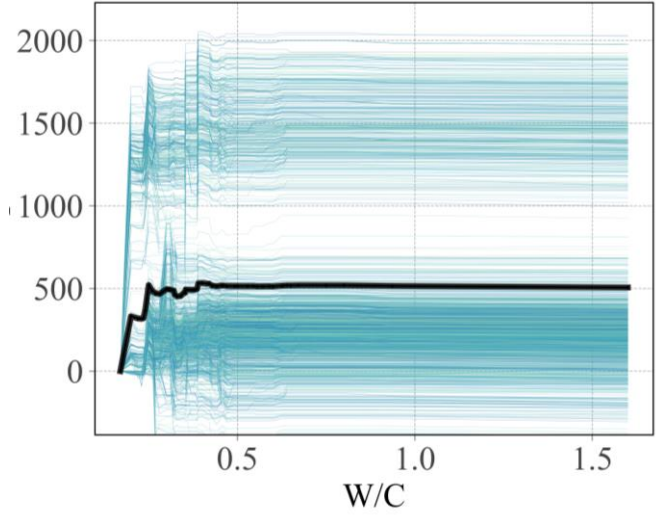
(c)



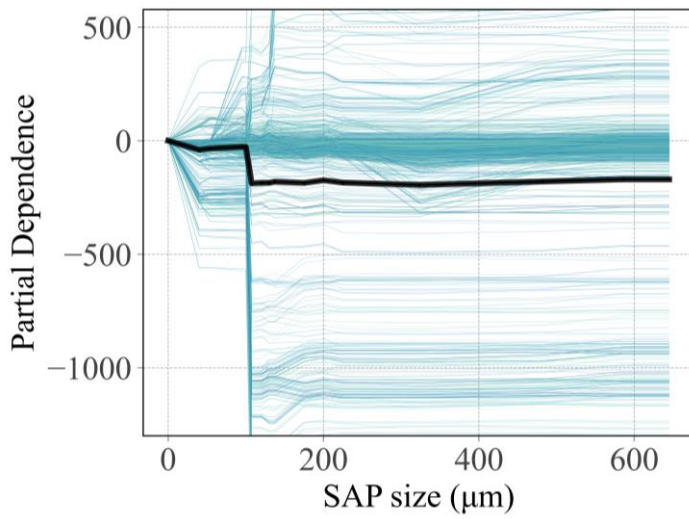
(d)



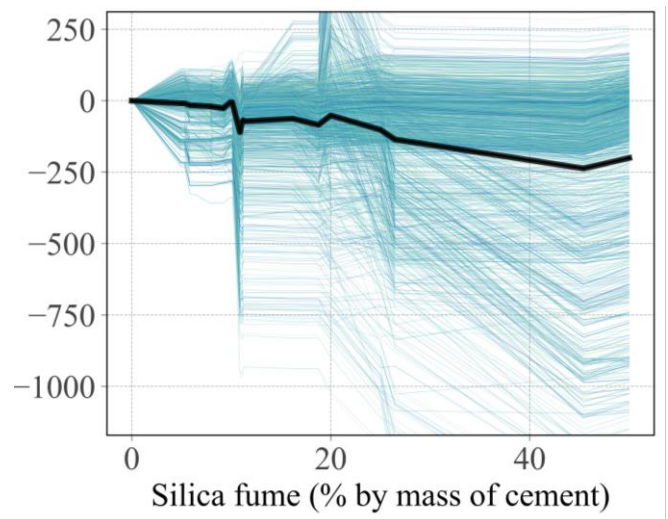
(e)



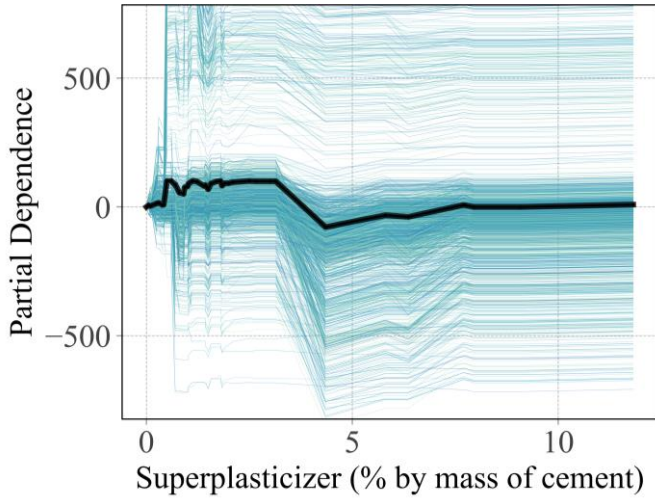
(f)



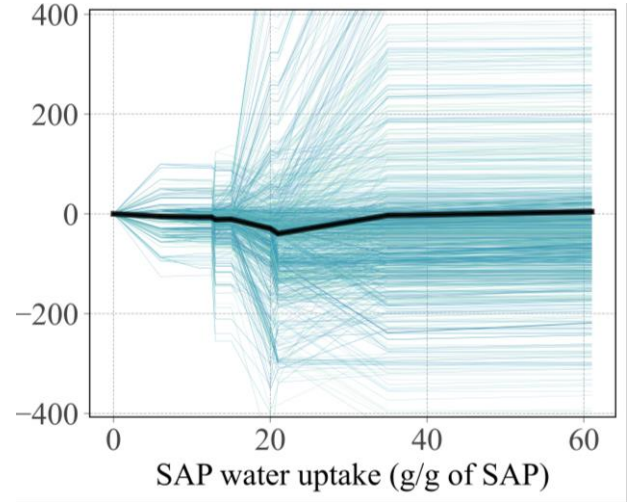
(g)



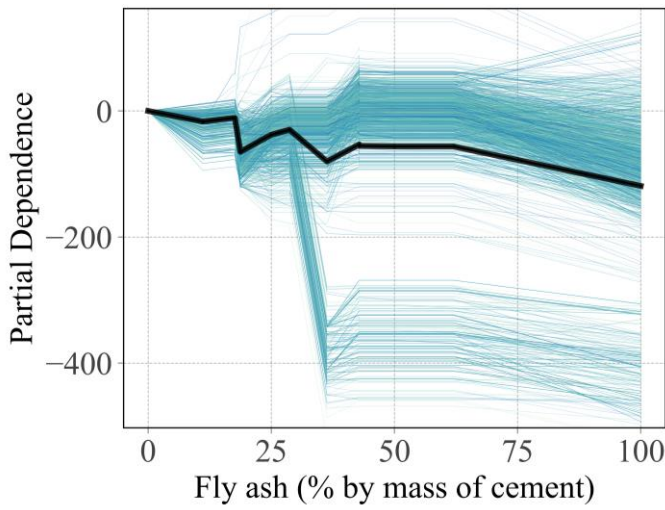
(h)



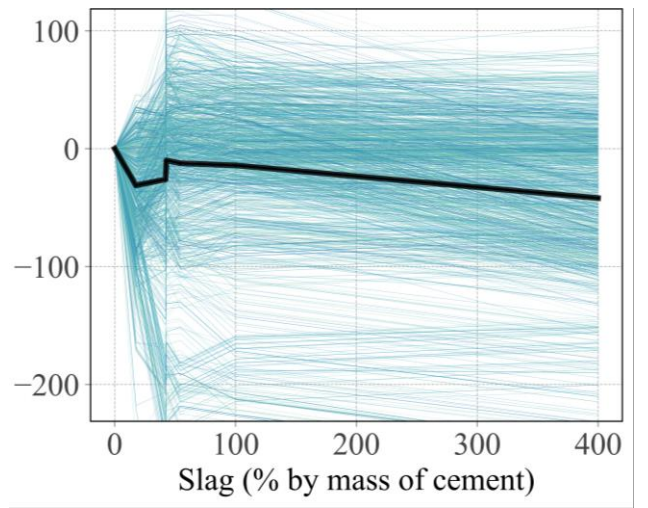
(i)



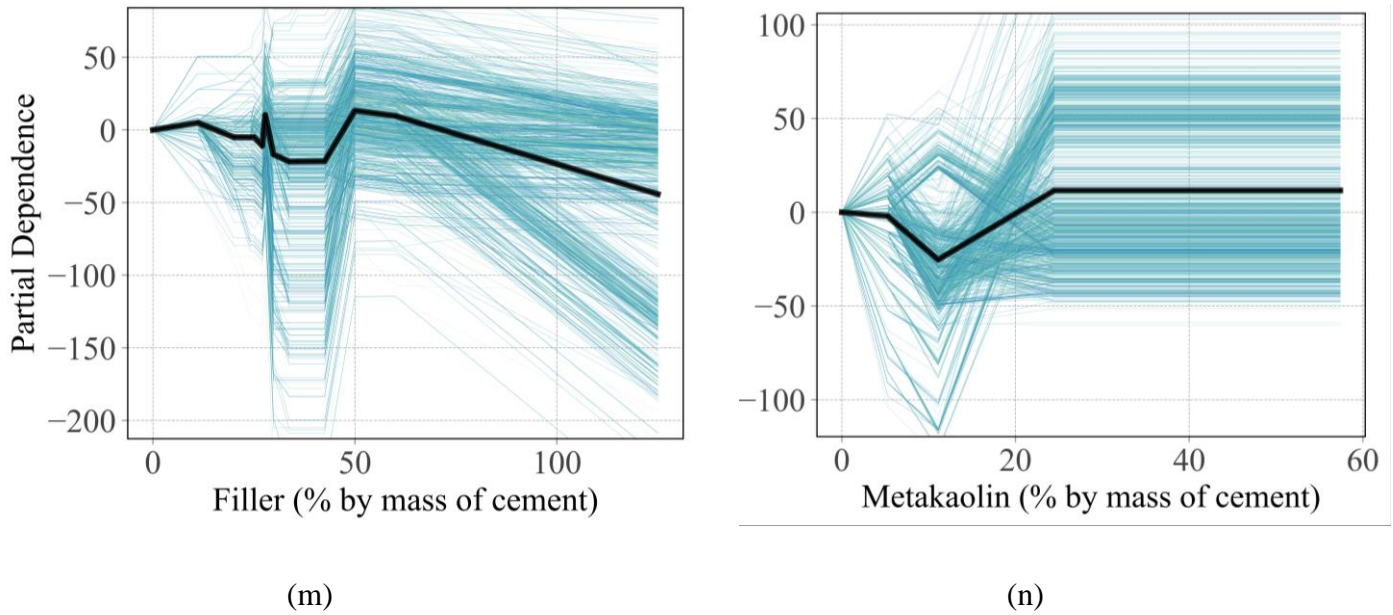
(j)



(k)



(l)



383 **Fig. 9.** Partial dependence plots (PDP 1D) analysis of the input variables effect on
 384 shrinkage/swelling of cementitious materials

385 The results of PDP 1D can be used for the preliminary study of concrete mix designs as the
 386 quick estimation of shrinkage/swelling can be performed with the help of figure 9. Indeed, using
 387 the initial mix composition, each graph in figure 9 can give a shrinkage/swelling gain value due to
 388 one parameter. For example, Table 3 illustrates the autogenous shrinkage/swelling values
 389 prediction at 1 and 2 days for three concretes with constant w/c of 0.25 incorporating three SAP
 390 contents (0%, 0.35%, and 0.7%). A w/b ratio of 0.25 leads to a gain value of 158 μe . This value is
 391 calculated relative to the minimum w/b ratio in the database (0.157), associated with a null gain
 392 since the higher the w/b ratio, the smaller the shrinkage. The A/C ratio of 2.82 is associated with
 393 a gain value of 304 μe because mortars and concretes shrink significantly less than pure cement
 394 paste, and cement content of 582 kg/m^3 gain is equal to -67 μe . SAP parameters exhibit similar
 395 gains in amplitude, thus consistently affecting predicted shrinkage/swelling values. In the end,
 396 predicted shrinkage/swelling values can be obtained by adding the mean shrinkage value (at 1 day)
 397 that is -280.93 μe and all the gains.

398

399 **Table 3.** Application PDP 1D in predicting shrinkage/swelling of the concrete W/B=0.25

	True mix design						Gain value according PDP plot					
W/B	0.25	0.25	0.25	0.25	0.25	0.25	158	158	158	158	158	158
A/C	2.82	2.82	2.82	2.82	2.82	2.82	304	304	304	304	304	304
Cement content	582	582	582	582	582	582	-67	-67	-67	-67	-67	-67
Fly ash content	0	0	0	0	0	0	0	0	0	0	0	0
Slag content	0	0	0	0	0	0	0	0	0	0	0	0
Silica fume content	0	0	0	0	0	0	0	0	0	0	0	0
Metakaolin content	0	0	0	0	0	0	0	0	0	0	0	0
Filler content	0	0	0	0	0	0	0	0	0	0	0	0
Superplasticizer content	1.4	1.4	1.4	1.4	2	2	10	10	10	10	10	10
SAP content	0	0	0.35	0.35	0.7	0.7	0	0	172	172	310	310
SAP size	200	200	200	200	200	200	-200	-200	-200	-200	-200	-200
Sap water uptake	13	13	13	13	13	13	0	0	0	0	0	0
Time	1	2	1	2	1	2	0	-58	0	-58	0	-58
	True swelling/shrinkage						Predicted= mean value (-280.93) + \sum Gain					
Shrinkage/Swelling	-171	-189.6	-19.6	-40.1	23.1	23.1	-75.9	-133.9	96.1	38.1	234.1	176.1

401 **5. Conclusions**

402 This study investigated the potential of machine learning models to predict the autogenous
 403 shrinkage of cementitious materials incorporating supplementary cementitious materials (SCM)
 404 and superabsorbent polymers (SAP). A new database has been built by combining shrinkage
 405 results reported in NU database and available studies dealing with the influence of SCM and SAP
 406 on autogenous concrete. Four machine learning models have been built: K-nearest neighbors
 407 (KNN), Random Forest (RF), Gradient Boosting (GB), and Extreme Gradient Boosting
 408 (XGBoost). The machine learning model performances have been studied using Monte-Carlo
 409 simulation. Shapley Additives Explanations (SHAP) and partial dependence plots were then used
 410 to interpret the machine learning models’ performance. The results have been discussed and
 411 compared to the available literature about autogenous shrinkage of cementitious materials with
 412 SCM and/or SAP. The following main conclusions can be drawn:

- 413 - A comprehensive database grouping 437 studies from the literature can be built (108
 414 shrinkage results published in articles related to shrinkage of cementitious materials with
 415 SAP, 142 shrinkage results from studies related to the effect of SCM on autogenous
 416 shrinkage, and 187 shrinkage values from NU database) and autogenous shrinkage values
 417 at 1 d, 2 d, 7 d, 14 d, and 28 d can be interpolated to generate a database containing 1889
 418 shrinkage values at different times with 14 parameters related to the concrete composition,

419 SAP content, SAP size and SAP water uptake. Specific attention has been devoted to
420 selecting diverse binary, ternary and quaternary experimental results within a broad range
421 of water-to-binder ratios.

422 - The machine learning models can achieve high training and testing accuracy on par with
423 neural network results published in the literature for predicting autogenous or drying
424 shrinkage.

425 - Two ensemble machine learning models, Random Forest (RF) and Extreme Gradient
426 Boosting (XGBoost), outperformed the other two models under investigation. This agrees
427 with previous machine learning models developed for cementitious materials.

428 - Through Monte Carlo simulation, the XGBoost model can achieve a high accuracy on the
429 training and testing sets, resp. $R^2=0.962$ and 0.954 . The predictions of machine learning
430 models are in good agreement with the experimentally measured values for
431 shrinkage/expansion values ranging from $-3800 \mu\epsilon$ (shrinkage) to around $1200 \mu\epsilon$
432 (expansion). XGB algorithms with default hyperparameters are suitable for building soft
433 computing tools in predicting the shrinkage/swelling of concrete containing SAP .

434 - The tuned models can be interpreted using SHAP values. The most influential parameters
435 were aggregate-to-cement (A/C) ratio, SAP content, time, water-to-binder (w/b) ratio,
436 water-to-cement ratio, cement content, and SAP size. The respective influences of these
437 parameters are consistent with experimental observations.

438 - Partial difference plots highlighted the influence of the parameters on the predicted
439 shrinkage values. It was found that shrinkage gradually decreases with increasing A/C and
440 w/b ratios between 0 and 5 and 0.2 and 0.4 resp., and SAP inclusion continuously reduces
441 shrinkage for content up to 0.6 % of cement mass.

442 The study might open up new research paths related to the optimal usage of SAP in
443 cementitious materials with SCM. For example, the results can guide the selection of concretes
444 constituents to decrease short-term autogenous shrinkage. Additions to the database are
445 encouraged to collaboratively build a more extensive database, including chemical descriptions of
446 SAP or shrinkage measurement methodology, for example. Possible developments can also be
447 envisioned by coupling the results reported herein and mechanical properties predictions. Such
448 advanced models might be of interest in the future regarding high or ultra-high performance eco-

449 friendly cementitious materials development.

450

451

452 **CRedit authorship contribution statement**

453 **Benoit Hilloulin:** Conceptualization, Methodology, Investigation, Formal analysis, Writing -original
454 draft, Writing - review & editing, Validation.

455 **Van Quan Tran:** Conceptualization, Methodology, Software, Visualization. Writing -original draft,
456 Writing - review & editing, Validation.

457 **Conflict of Interest:** The authors declare that there is no conflict of interest.

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459 commercial, or not-for-profit sectors.

460 **Availability of data and material:** Data is provided as supplementary data.

461

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