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Interpretable Machine Learning Model for Autogenous Shrinkage Prediction of Low-Carbon Cementitious Materials

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Highlights

- A large database about the autogenous shrinkage of concrete with SCM is built
- Ensemble machine learning models can predict the autogenous shrinkage efficiently
- ML models can perform better than B4 and CEB models modified versions.
- SCM influence can be interpreted using SHAP analysis
- Insights into blended cement concrete shrinkage behavior can be envisioned.

Abstract

Supplementary cementitious materials (SCM) are key components of low-carbon cementitious materials. However, their effects, especially for the emerging high cement replacement ratio formulations, are sometimes very challenging to predict, leading to restrictions in most standards. Through advanced Machine Learning techniques, this study provides novel insights into the autogenous shrinkage properties of concrete containing various kinds of supplementary cementitious materials such as slag, fly ash, silica fume, calcined clay, and filler. Four machine learning models are optimized and their predictions are compared on a dedicated database, including ternary and quaternary cement blends. The Extreme Gradient Boosting (XGBoost) model exhibited the highest accuracy among these models. Interpretative tools such as SHAP analysis are then used to obtain novel information about the relative influence of the SCM on the autogenous shrinkage depending on their dosage. The model is finally compared to the recently modified versions of the B4 and the CEB analytical models to predict the autogenous shrinkage of unknown concrete formulations. The model showed significantly better predictions than the analytical models, and a web application is proposed, paving the way for precise and

30 interpretable autogenous shrinkage predictions of cementitious materials incorporating SCM.

31

32 Keywords: Concrete; Autogenous Shrinkage; Supplementary Cementitious Material (SCM);
33 Machine Learning; XGBoost; Shrinkage Models.

34

35 **1 Introduction**

36 Decreasing cementitious materials' carbon footprint is necessary to limit the overall
37 environmental impact of the construction industry. This decrease can be achieved through several
38 techniques such as the construction and demolition waste (CDW) usage, for example, the use of
39 crushed concrete waste into Recycled Aggregate Concrete (RAC) [1], or the extensive use of
40 supplementary cementitious materials, some of them being industrial byproducts [2–4]. However,
41 these additions considerably impact the behavior of cementitious materials, and, because of these
42 rapid evolutions, such novel components are rarely very well understood nor precisely considered
43 in the construction standards. More specifically, it is generally admitted that concrete early age
44 deformations can induce severe structural evolutions. Apart from environmental degradations,
45 these deformations are mostly due to shrinkage and creep mechanisms [5]. For example, high-
46 performance and ultra-high performance concrete (HPC and UHPC) exhibit significant early age
47 deformations because of their low water-to-cement ratio. Indeed, while deformation of normal
48 strength concrete is primarily governed by drying shrinkage, which occurs some weeks or months
49 after setting due to a water loss, deformation in low water-to-cement concrete can develop very
50 quickly at an early age because of the rapid evaporation of water from the surface of the specimen,
51 namely plastic shrinkage, or because of the consumption of water during the hydration directly
52 causing chemical shrinkage, and generating capillary depressions leading to macroscopic
53 deformations referred to as autogenous shrinkage. It has been found that autogenous shrinkage can
54 represent more than half of the total deformation in ultra-high performance concrete [6], creating
55 considerable stresses at a microscale that can lead to cracking. As cracking should generally be
56 avoided, either because of structural concerns or aesthetic reasons[7,8], specific attention should
57 be paid to early-age deformation of low water-to-cement ratio high and ultra-high performance
58 concrete.

59 Several analytical models have been introduced during the last decades to predict shrinkage.
60 The major construction codes provide quick ways to estimate the shrinkage amplitude of several

61 concrete mixes based on their composition and, in some cases, by considering standard strength
62 characteristics such as the 28-days compressive strength. Power and exponential laws have been
63 introduced to describe the shrinkage amplitude evolution relatively to time [9,10]. Thanks to these
64 laws, the quick increase in autogenous shrinkage amplitude during the first weeks can be grasped.
65 Most of these models are a combination between empirical laws and advanced theories. For
66 example, B4 model [10] is supported by the solidification theory, the theory of microprestress
67 relaxation, activation energy concepts, the moisture diffusion theory, and damage models for
68 microcracking, and proved very good results in predicting autogenous and drying shrinkage of
69 structural elements [11]. Other models have been proposed in reference codes such as Eurocode 2,
70 fib CEB MC 10 [9,12,13]. Recent improvements of both the B4 and the CEB MC 10 model have
71 been proposed to take into consideration the influence of some supplementary cementitious
72 materials [14,15]. These models have been found particularly effective in predicting long-term
73 predictions deformation of concrete, but several shortcomings have been noticed concerning early-
74 age prediction and regarding actual concrete formulations, which can include a high proportion of
75 additions [15,16]. Moreover, the growing use of various supplementary cementitious materials
76 (SCM), leading to ternary or quaternary concrete mixes in which synergistic effects may arise, is
77 rarely taken into consideration.

78 Indeed, due to economic and environmental considerations, an increasing amount of SCM is
79 being used in recent concrete formulations. Various SCM such as calcined clay, fly ash, ground
80 granulated blast furnace slag, later referred to as slag, and silica fume commonly replace cement,
81 while additions like fillers may partially replace cement or only play a physical role in increasing
82 the overall compacity of the mix. These additions influence shrinkage mechanisms to various
83 extents, especially autogenous shrinkage. It is commonly admitted that silica fume, commonly
84 used in UHPC due to its filling properties and high pozzolanic activity, increases shrinkage even
85 for small replacement ratios [5]. Conversely, fly ash alone has been reported to decrease shrinkage
86 in most studies because of the slower hydration reaction [17,18]. In most published studies, slag
87 increased autogenous shrinkage, especially long-term autogenous shrinkage, because its fineness
88 leads to high reactivity and higher chemical shrinkage than pure cement concrete [19–22]. Some
89 uncertainty remains concerning the influence of slag on the autogenous shrinkage of UHPC since
90 it has been reported that the addition of slag increased the autogenous shrinkage in some cases
91 [15]. With the demand for low-cement concrete, calcined clay, which is readily available around
92 the globe, has been proved to be an interesting product to cut CO₂ emissions due to concrete

93 formulation. Though calcined clay, generally associated with limestone to produce LC³ cement,
94 induces novel chemical reactions during hydration, and leads to a fine porosity [23], its influence
95 on the autogenous shrinkage is rarely reported and might not be prejudicial [24–26]. Finally, fillers
96 have been found to decrease shrinkage as they act like small aggregates restricting deformations
97 [27,28], but their interactions with other additions are often only considered from a chemical point
98 of view and are rarely addressed from a shrinkage point of view [27,29].

99 Therefore, with the increasing complexity of concrete formulations, a better understanding of
100 fundamental evolutions such as autogenous shrinkage is needed. Recent studies have proposed
101 adaptation to the aforementioned analytical models to consider the use of SCM and their eventual
102 combination [15,30]. In [15], CEB Model Code 2010 has been improved by introducing correction
103 factors using an extensive experimental campaign. However, such parameters might not represent
104 other concrete formulation behaviors, and more extensive shrinkage databases should be built.

105 Recent developments in Machine Learning (ML) have provided novel insights into concrete
106 properties-related issues [31]. Since the publication of the first Artificial Neural Network model
107 (ANN) to predict concrete compressive strength [32], numerous research works have been
108 published to predict concrete compressive strength with ML-based models [33–36]. ML-based
109 models have also proved their interest in predicting other concrete properties such as fresh
110 properties [37], creep [38,39], chloride [40], carbonation resistance [41], frost resistance [42] and
111 shrinkage [43,44]. They can also be used for microscale properties determination and
112 enhancement, such as during indentation [45,46], image analysis [47–50], or large-scale structural
113 monitoring [51,52]. While ML models might have initially appeared as black-box models, recent
114 advances such as features analysis and dubbed SHapley Additives exPlanations (SHAP)
115 introduced novel ways to explore the impacts of the model inputs on the final predictions [53].
116 Such tools have been used recently in several studies related to concrete [44,54] and might help
117 build advanced autogenous shrinkage prediction models comparable to the existing most
118 performant analytical models such as B4 and CEB models.

119 This study develops an interpretable ensemble ML model to predict the autogenous shrinkage
120 evolution in low-carbon cementitious materials with SCM. An extensive dedicated database is
121 built, including ternary and quaternary formulations, and optimized ML models are compared to
122 the classic and improved versions of B4 and CEB Model Code models using interpretative tools
123 such as SHAP. Then, a web application is proposed to provide fast and precise shrinkage

124 predictions to the Civil Engineering community. The manuscript is structured as follows: a first
125 section describes the new shrinkage database developed during this study, then a section presents
126 the numerical methods employed before analyzing and discussing the results and a conclusion.

127

128 **2 Autogenous Shrinkage Database description and analysis**

129 To develop an accurate model for autogenous shrinkage prediction of concrete incorporating
130 SCM, a comprehensive experimental database is required. To this end, we adopted the method
131 published in [44]. The original NU database containing various creep and shrinkage evolutions of
132 cementitious materials has been extended by low water-to-cement ratio cement paste, mortar or
133 concrete samples autogenous shrinkage curves. This database has been further extended to include
134 more autogenous shrinkage data of various concrete of binary, ternary or quaternary formulations
135 from various sources [15,26,55–60]. In total, a database comprising 347 autogenous shrinkage
136 observations and 28d compressive strength of various concrete mixes has been built. To the authors
137 knowledge, this is the most comprehensive autogenous shrinkage database to date. The final
138 database covers a wide range of water-to-cement and water-to-binder ratios (from normal strength
139 to ultra-high strength concrete) as well as a wide variety of binary, ternary and quaternary
140 formulations. These shrinkage curves were interpolated to obtain 1d, 2d, 7d, 14d, and 28d
141 shrinkage values. Twelve input variables have been considered: water-cement ratio (W/C), water-
142 binder ratio (W/B), aggregate-cement ratio (A/C), cement content (kg/m^3), silica fume content (%
143 cement mass), fly ash content (% cement mass), slag content (% cement mass), calcined clay
144 content (% cement mass) (denoted as metakaolin content), filler content (kg/m^3), amount of
145 superplasticizer (% cement mass), time since the beginning of shrinkage measurements (days) and
146 28-d compressive strength (MPa). After removing data points with missing data, a database with
147 1482 datapoints has been finally obtained. The descriptions and statistical attributes of the input
148 variables are given in Table 1, and Fig. 1 displays their statistical distributions. It can be seen that
149 a wide range of compositions has been investigated as water-to-binder ratios range from 0.16 to
150 0.86, cement content ranges from $167.4 \text{ kg}/\text{m}^3$ to $1632 \text{ kg}/\text{m}^3$ (cement paste) with a large
151 proportion of values between $167 \text{ kg}/\text{m}^3$ and $700 \text{ kg}/\text{m}^3$ for concretes. Supplementary cementitious
152 materials contents reflect the actual wide variety of formulations, some of them with important
153 substitution amounts. Indeed silica fume content, fly ash content, slag content, calcined clay and
154 filler content up to 50%, 150%, 400%, 57.4% and 125% relatively to cement mass were

155 considered. A maximum shrinkage value of around $-2089 \mu\epsilon$ has been obtained and a median
 156 shrinkage value of $-114.7 \mu\epsilon$ can be calculated. Common autogenous shrinkage features can be
 157 retrieved from the 2D scatter plots exposed in Fig. 1 by plotting linear regressions: shrinkage
 158 increases with smaller W/B and A/C values, while it generally increases with higher cement or
 159 silica fume content as well as higher compressive strength as they are generally associated to low
 160 W/B values.

161 Correlations between the model parameters were calculated too. Fig. 2 gives a graphical
 162 representation of the correlation matrix. As expected, strong positive correlations can be observed
 163 between, W/B, A/C and shrinkage, and strong negative correlations can be observed between
 164 shrinkage and fc_{28} , cement content or silica fume content. However, no strong correlations
 165 between input variables, and as such, all these variables were used as the input for ML.

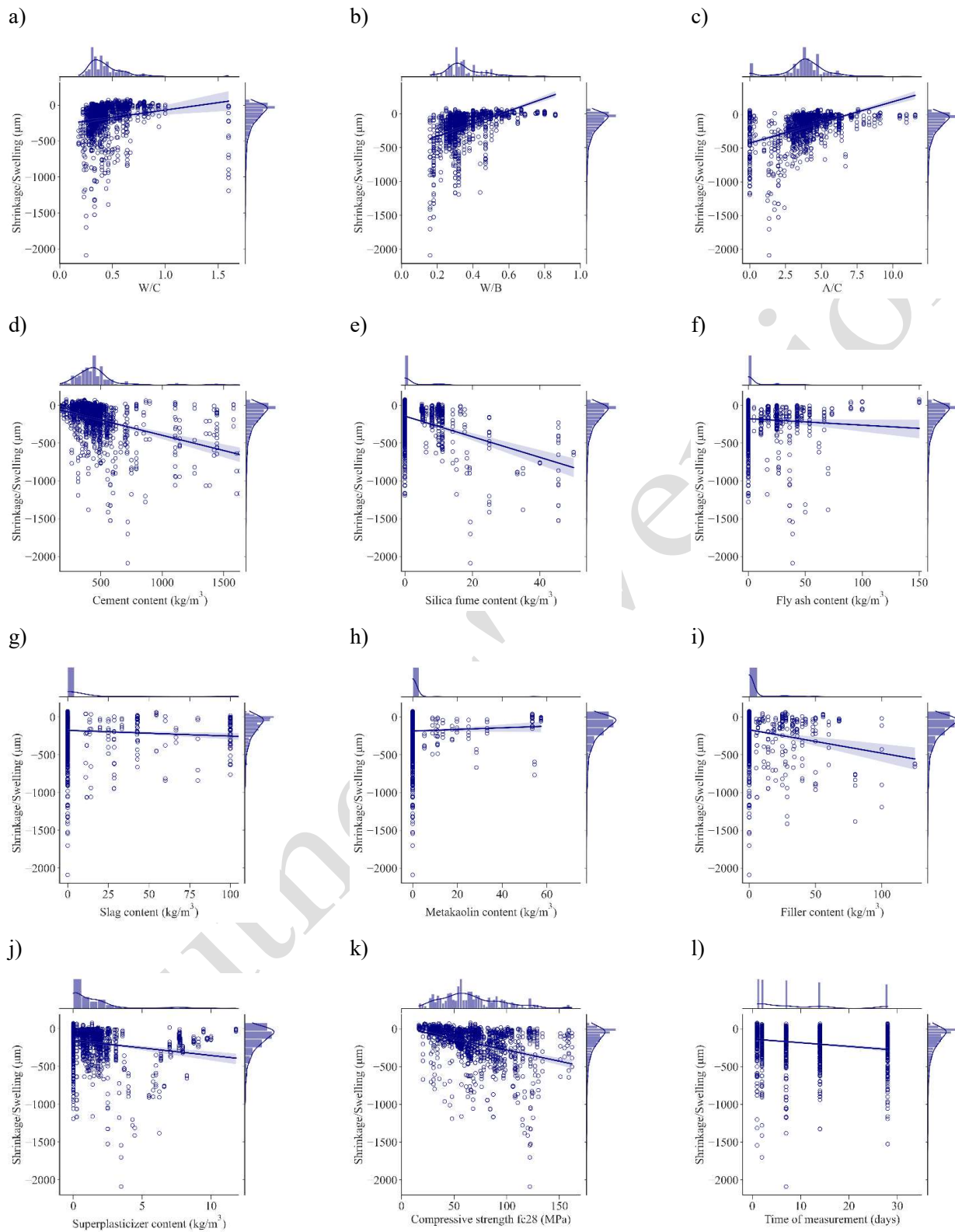
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167 **Table 1.** Description of the database used in this study

	Unit	Min	Q25%	Mean	Median	Q75%	Max	Std	Skw
W/C	-	0.180	0.320	0.444	0.390	0.500	1.600	0.188	2.807
W/B	-	0.160	0.290	0.360	0.336	0.400	0.860	0.117	1.295
A/C	-	0.00	3.28	3.90	3.90	4.73	11.56	1.77	0.36
Cement content	kg/m ³	167.4	360.0	472.1	440.0	496.0	1632.0	222.3	2.9
Silica fume content	% cem	0.0	0.0	3.0	0.0	0.0	50.0	7.2	3.7
Fly Ash	% cem	0.0	0.0	8.2	0.0	0.0	150.0	18.3	3.1
Slag content	% cem	0.0	0.0	9.8	0.0	0.0	400.0	40.6	6.7
Metakaolin content	% cem	0.0	0.0	1.6	0.0	0.0	57.4	8.2	5.7
Filler content	% cem	0.0	0.0	4.7	0.0	0.0	125.0	14.5	4.1
Superplasticizer content	% cem	0.0	0.0	1.5	0.8	1.8	11.8	2.2	2.3
Compressive strength fc_{28}	MPa	16.5	45.9	67.1	63.0	85.7	162.0	29.4	0.8
Time of measurement	days	1.0	2.0	9.7	7.0	14.0	28.0	9.6	1.0
Shrinkage/Swelling	$\mu\epsilon$	-2089.600	-243.000	-182.832	-114.700	-28.650	78.900	237.617	-2.576

168 Skw=Skewness; Std=Standard deviation;

169



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

171

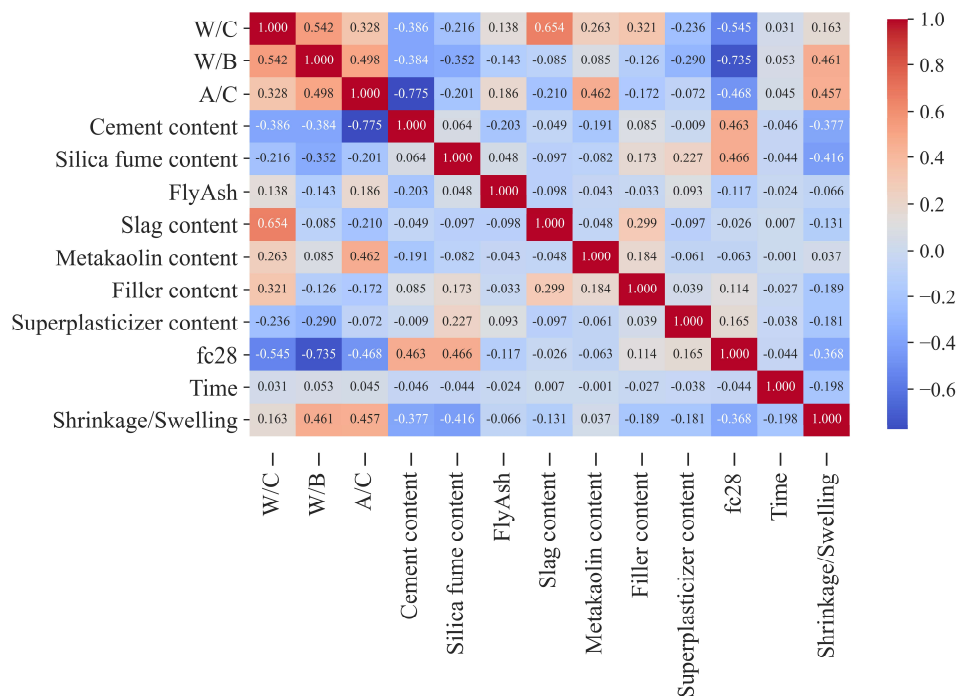


Fig. 2. Pearson correlation of all feature and Shrinkage/Swelling

3 Shrinkage prediction using Machine Learning and Analytical models

3.1 Modeling strategy

The modeling strategy is four steps presented in Figure 3:

- Step 1: Collection a database consisting 12 input variables and one output variable “shrinkage/swelling”.
- Step 2: Determination the best performance of ML model

All the observation data from the original database have been classically split into training and testing datasets. 70% of whole dataset is used to building the four ML models including SVM, ANN, GB and XGB with aided of metaheuristic optimization algorithm Simulated Annealing (SA) Optimization algorithm which tunes the hyperparameters of four ML algorithms. The K-Fold Cross Validation (CV) is integrated in the tuning hyperparameter process for validating the cost function R^2 of optimization process. The evaluation ML performances are carried out with aided of three metrics, such as R^2 , RMSE and MAE, in prediction of Shrinkage/Swelling. Based on the best performance, the best ML model is proposed for the next steps.

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- Step 3: Interpretation of XGB black box with SHAP value
- In this step, the SHAPley Additive exPlanations (SHAP) [61] based on the best ML model is used for the interpretation of predicted Shrinkage/swelling values. The effect of each feature is quantified by SHAP global and SHAP local.
- Step 4: Comparison of predicted value based on the best ML model with B4 and CEB analytical models

The concrete formulations in the original database have been divided into a training and a test set to guarantee that no shrinkage value from any concrete with all time of measurement in the test set is known. Then the best Machine Learning model is fitted on this training set, and its performance is compared to the performance of the analytical models on the test set.

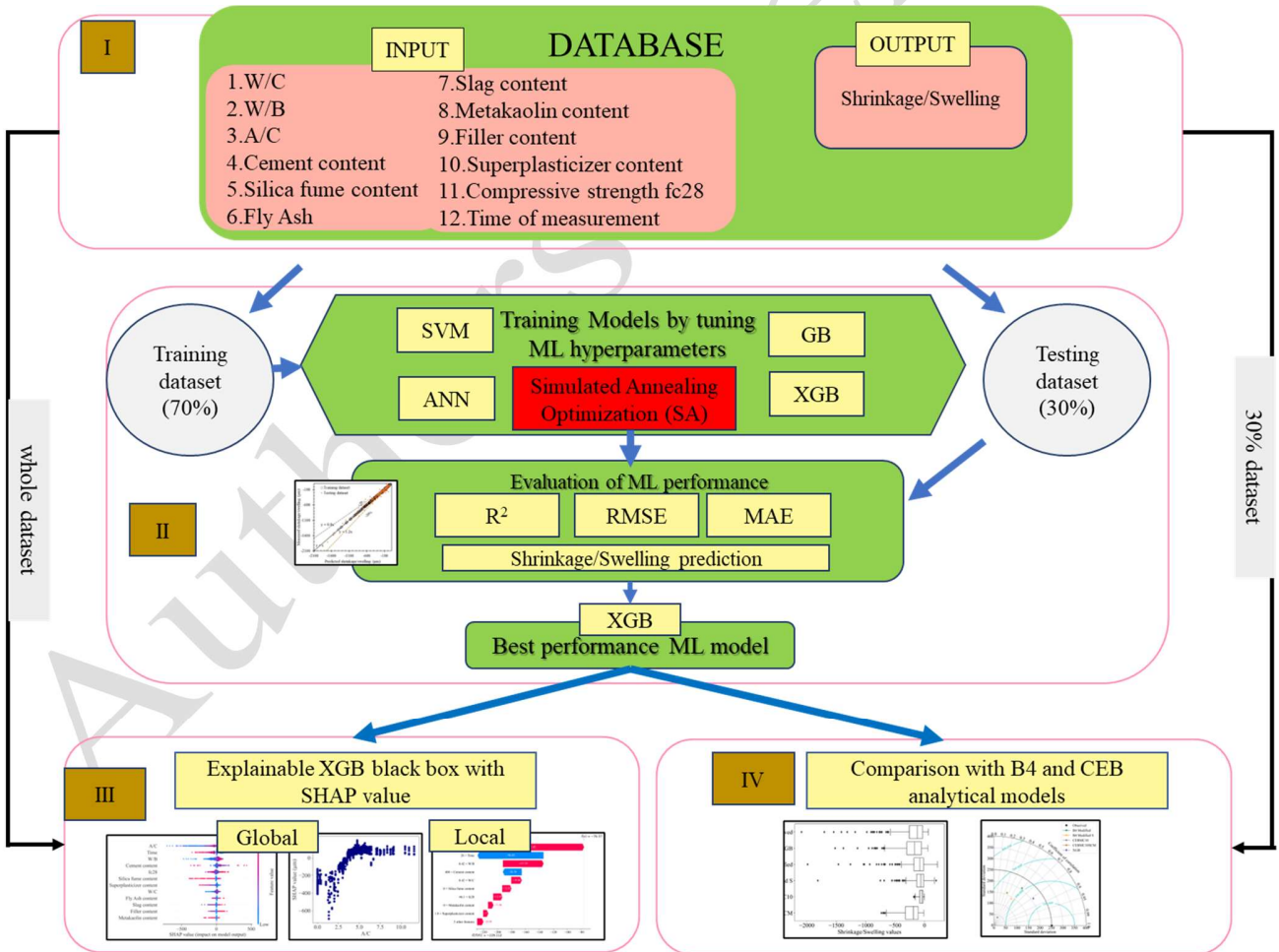


Fig 3. Conception of shrinkage/swelling investigation

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205 3.2 Machine learning models

206 3.2.1 Support Vector Machine (SVM)

207 The support vector machine algorithm introduced by Vapnik [62] can be used to address
208 classification difficulties. For the solution of regression and prediction issues, the support vector
209 machine was further modified and dubbed support vector machine regression (SVR) [63]. The SVR
210 method sought to reduce the generalization error and get the best solution using the structural risk
211 minimization concept. The Gaussian radial basis function was used in this work to transition from
212 a lower-dimensional feature space to a higher one, allowing for linear regression and improved
213 fitting of the training dataset. The following linear function can be used to represent the output
214 variable:

$$f(x) = \langle \omega \cdot \varphi(x) \rangle + b \quad (1)$$

215 where $\langle \cdot \rangle$ denotes the dot function; $\varphi(x)$ is a transformation that translates the input feature to a
216 higher dimensional feature space; b is the function's parameter vector (model bias); ω are the
217 minimum values derived from the following equation:

$$\text{minimise } \left[\frac{1}{2} \|\omega\|^2 + C \sum_{j=1}^n (\xi_j + \xi_j^*) \right] \quad (2)$$

$$\text{considering } \begin{cases} y_j - \omega \cdot \varphi(x_j) - b \leq \varepsilon + \xi_j \\ \omega \cdot \varphi(x_j) + b - y_j \leq \varepsilon + \xi_j^* \\ \xi_j, \xi_j^* \geq 0 \end{cases} \quad (3)$$

218 where ξ_j, ξ_j^* are the slack variables; C is the regularization parameter; ε is the insensitive loss function
219 (error between the test and forecast values); y_j is the test result; and n is the sample size.

220

221 3.2.2 Artificial Neural Network (ANN)

222 The most widely used machine learning model is ANN, which is based on biological neural
223 networks. It is made up of input neurons (similar to synapses), multiplied by weights representing
224 the intensities of the relevant impulses, and then determined by the neuron's activation function.
225 Finally, the required result will be computed by another function (perhaps an identity function). It
226 is feasible to acquire the output matching to certain inputs by altering the weight of the artificial
227 neuron. However, when there are too many neurons, calculating these weights becomes problematic.
228 At this time, numerous ways are being developed to modify the weights of the neurons in order to
229 get the output as rapidly as feasible. In this study, the solver for weight optimization contains three
230 methods including 'LBFGS' Limited-Memory Broyden-Fletcher-Goldfarb-Shanno method of
231 quasi-Newton methods, 'SGD' refers to stochastic gradient descent and the last 'ADAM' referring

232 to a Stochastic Gradient-Based Optimizer proposed by Kingma et al. [64]. In this investigation, the
 233 best optimization solver will be selected by the metaheuristic algorithm in the process of tuning
 234 hyperparameters.

235

236 3.2.3 Gradient Boosting (GB)

237 Gradient Boosting (GB) improves predictions by using a method called as augmentation.

238 The algorithm in boosting attempts to examine and correct predictions that are not acceptable on the
 239 first iteration [65]. The algorithm's iterative process for correction then continues until the desired
 240 prediction is obtained. Increased assistance for decreasing bias and variation in order to strengthen
 241 poor learners.

242 Gradient Boosting is the process of combining several weak predictive models into a single
 243 strong model [66]. In this case, a poor prediction model may perform somewhat better than random
 244 guesses.

245 The model using the Boosting ensemble learning strategy can be expressed as follows:

$$F_N(x) = \sum_{n=1}^M \alpha_n f_n(x) \quad (4)$$

246 The ensemble learning model $F_N(x)$ is generated by the linear combination of N basic
 247 learning machine models, where $f_n(x)$ represents the mth basic learning machine and n represents
 248 the weight of the nth basic learning machine.

249 The gradient boosting algorithm operates on the gradient descent approach, which is based
 250 on the functional. To begin, the goal function is as follows:

$$E = \sum_{t=1}^T L(y_t, F_N(x_t)) = \sum_{t=1}^T L(y_t, \alpha_n \times f_n(x_t)) \quad (5)$$

251 The number of samples is T, the number of basic learning machines is N, and the loss
 252 function is L. The training procedure is to train each basic learning machine f_n , n-1, 2,..., N in turn
 253 so that the objective function value E is the smallest, that is, the training outcomes for the nth basic
 254 learning machine are as follows.

$$\sum_{t=1}^T L(y_t, F_{n-1}(x_t) + \alpha_n \times f_n(x_t)) \cong \sum_{t=1}^T L\left(y_t, F_{n-1}(x_t) + \sum_{t=1}^T \frac{\partial L}{\partial F_{n-1}(x_t)} \times f_n(x_t)\right) \quad (6)$$

255 According to the principle of gradient descent, the optimal model should be the negative
 256 gradient direction of the objective function, that is:

$$f_n^*(x) = \arg \min_{f, \alpha} \sum_{t=1}^T L \left(-\frac{\partial L}{\partial F_{n-1}(x_t)} - \alpha \times f(x_t) \right)^2 \quad (7)$$

257 After obtaining the best A, coefficient S can be found by minimizing the objective
 258 function, namely:

$$\alpha_n^* = \arg \min_{\alpha_n} \sum_{t=1}^T L(y_t, F_{n-1}(x_t) + \alpha_n \times f_n^*(x_t)) \quad (8)$$

259 The preceding steps are repeated until all N basic learning machines and coefficients have
 260 been trained, and a learning model based on Equation 1 has been generated. The gradient boosting
 261 approach is used in the learning model, and the next fundamental machine learning model may
 262 further increase the accuracy based on the previous underlying machine learning models, reducing
 263 the model's deviation. This is the distinction with the Bagging. Basic machine learning can be a low-
 264 accuracy model; through the improvement approach, the accuracy of the entire model can be
 265 steadily increased, but there is a certain degree of fit at the same time.

266

267 3.2.4 Extreme Gradient Boosting (XGB)

268 The Extreme Gradient Boosting (XGB) algorithm is a cutting-edge method for solving
 269 supervised learning problems with high precision [26]. If Deep Learning only accepts raw data in
 270 numerical form (which must typically be converted to n-vectors in the real number space), XGB
 271 accepts tabular datasets of any size, including categorical data. Furthermore, XGB has a rapid
 272 training speed, can scale for parallel computing on several servers, and can be GPU-accelerated,
 273 therefore Big Data is not an issue for this model. The earliest and most well-known model of the
 274 most recent generation of tree booster ensembles is the XGB; a representation of this approach is
 275 the Gradient Boosting Decision Tree (GB) or Multiple Additive Regression Tree (MART).

276 The basic idea behind XGB is to first train a tree with the training set and the real value of
 277 the sample (i.e. the standard response), and then use that tree to forecast the training set to acquire
 278 the proper value. The residuals are the predicted value of each sample, as well as the difference
 279 between the forecast and the real value. The second tree is then trained, but this time instead of using
 280 the real number, use the residual as the standard response. After training two trees, the residuals of
 281 the sample can be used to train more trees. To stop training, the total number of trees can be selected
 282 explicitly or based on particular indicators.

283 The XGB algorithm can be thought of as a K-tree additive model:

$$\hat{y}_i = \sum_{k=1}^K f_k(x_i), f_k \in F \quad (9)$$

284 The gradient boost model does not learn the weights of the d-dimensional space but directly
 285 learns the decision tree set, where F is a function space consisting of all trees (here the regression
 286 tree is also a partial function and the varied values of the different portions form a tree). The
 287 objective function of XGB is a sum of a particular loss function assessing overall predictions and a
 288 sum of all predictors' regularization terms (K trees).

289 Mathematically:

$$obj(\theta) = \sum_i^n l(y_i - \hat{y}_i) + \sum_{k=1}^K \Omega(f_k) \quad (10)$$

290 Where l is the loss function, which is the difference between the expected and actual outputs \hat{y}_i and
 291 y_i . While Ω is a measure of how complicated the model is, it aids in preventing model over-fitting and
 292 is determined using:

$$\Omega(f_k) = \gamma T + \frac{1}{2} \lambda \|w\|^2 \quad (11)$$

293 The number T in the preceding equation reflects the number of leaves on the tree, and w
 294 represents the weight of each leaf.

295

296 3.2.5 Simulated Annealing Optimization algorithm (SA)

297 Kirkpatrick et al. [67] pioneered simulated annealing (SA) in 1983. This metaheuristic
 298 method is based on physical phenomena seen in continuum mechanics. To avoid becoming stuck in
 299 local minima, SA employs a random search engine represented by Markov chains. SA employs
 300 solution variants to increase the objective function while still maintaining the solutions, albeit the
 301 least efficient, within specified constraints. Any adjustment that improves the objective function, J,
 302 is permitted in the minimization problem; however, candidates that raise J are also included in the
 303 solution set with probability p, which is known as the transition probability [68]:

$$p = \exp\left[-\frac{\Delta E}{k_B T}\right] \quad (12)$$

304 where k_B is Boltzmann's constant, T is the annealing process temperature, and E is the energy level,
 305 is connected with the goal function modification by the constant, [68].

$$\Delta E = \gamma \Delta J \quad (13)$$

306 A random threshold, r , such that $p > r$, determines whether a solution modification is
 307 acceptable. T lowers and the system cools down during optimization. A high T indicates a high-
 308 energy system that is difficult to reduce, whereas a low T indicates a low-energy system that may
 309 be trapped in a local minimum [69]. The proper decision T may be to first search the space for the
 310 global minimum and then, as the system cools down, converge to a solution with sufficient accuracy
 311 [68]. Stopping conditions, such as limiting the number of repeats or focusing on the improvement
 312 of the goal function, are incorporated in t_f [70].

313

314 3.2.6 Performance evaluation of models

315 In order to evaluate the performance of ML models, three popular statistical metrics, such as
 316 coefficient of determination R^2 , Root Mean Square Error (RMSE), and Mean Absolute Error
 317 (MAE), are introduced in following:

$$R^2 = \frac{\sum_{j=1}^N (p_{0,j} - \bar{p}_0)(p_{t,j} - \bar{p}_t)}{\sqrt{\sum_{j=1}^N (p_{0,j} - \bar{p}_0)^2 \sum_{j=1}^N (p_{t,j} - \bar{p}_t)^2}} \quad (16)$$

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{j=1}^N (p_{0,j} - p_{t,j})^2} \quad (17)$$

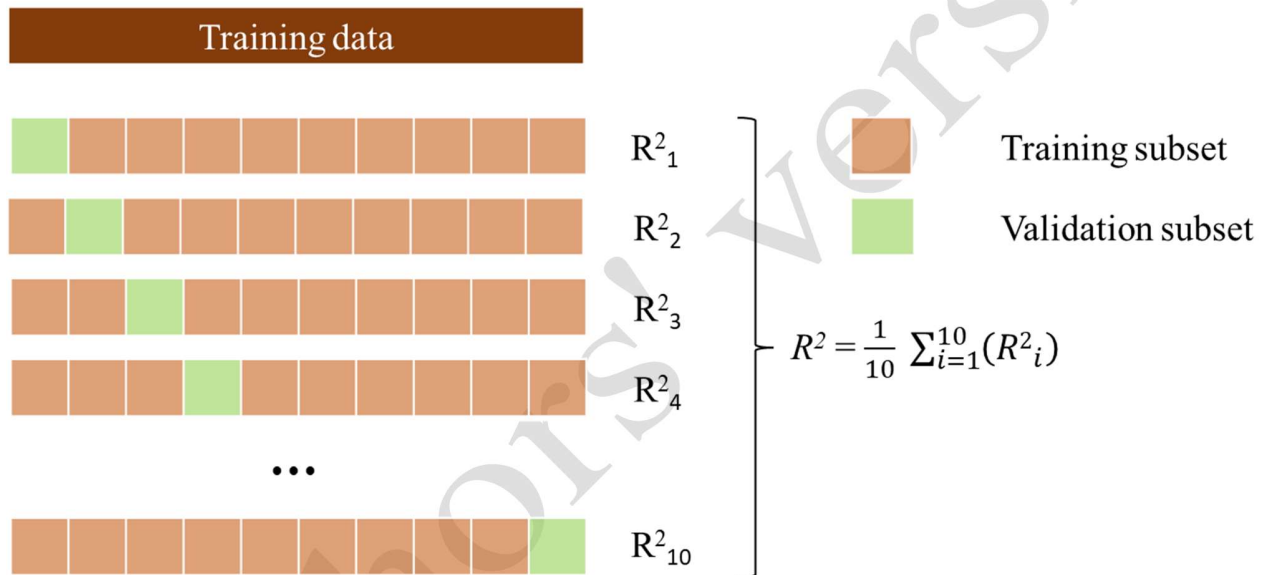
$$\text{MAE} = \frac{1}{N} \sum_{j=1}^N |p_{0,j} - p_{t,j}| \quad (18)$$

318 Where $p_{0,j}$ is the shrinkage/expansion value of the i -th sample point in the database; $p_{t,j}$ is
 319 the machine learning model prediction value for the i -th sample point; \bar{p}_0 is the averaged
 320 experimental value of shrinkage/expansion; and \bar{p}_t is the mean predicted value. Both MAE and
 321 RMSE explicitly quantify the residual error at each sample point and thus provide an accurate
 322 assessment of model performance. R^2 normalizes the squared residual error with the database
 323 variance and generates dimensionless values ranging from 0 to 1. Because RMSE is often seen to
 324 be more understandable because it is equivalent to measured values and handy for comparing the
 325 performance of different models, it was chosen as the primary metric index.

326 **3.2.7 K-Fold Cross Validation technique**

327 To tune hyperparameters in machine learning algorithms, K-fold cross-validation (CV) is
 328 utilized. Choosing k affects the variance; a low k value results in significant variance or bias.
 329 Furthermore, while deciding on k, the data quantity and computational capabilities of the system
 330 must be taken into account. The value of k in this study is set to 10 [71,72], indicating that the number
 331 of training and testing rounds is ten. The dataset is split into two parts: training and testing. The
 332 training data area is partitioned into k sections of equal size. The model is then trained with different
 333 hyperparameters on k-1 subsets and evaluated on the last subset. The process is repeated k times
 334 before averaging the evaluation results as illustrated in Figure 4.

335



336

337 **Fig 4.** 10-Fold CV of training dataset with cost function of R^2 coefficient of determination

338

339 **3.3 Comparison with Analytical Models**

340 Three analytical models are also adopted for comparison to examine the prediction accuracy
 341 of the machine learning models detailed above. These models are the B4 model [10], CEB MC 10
 342 [9] model and a modified version of CEM MC 10 model to include the effect of SCM which has
 343 been introduced recently [15] and will be referred to as 'CEBMC10SCM' model in this study. The
 344 autogenous shrinkage model prediction are given as follows:

- 345 • Modified B4 model [73]:

346 Using this composition-based model, the autogenous shrinkage can be calculated at any time:

$$\epsilon_{au}(t) = k_{\gamma} k_s C t^n \quad (19)$$

347

348 where k_{γ} depends on the cement type, $k_s = \left\{ 1 + 3 \left(\frac{SiO_2}{Cement} \right) \right\} \left\{ 1 + 2 \left(\frac{Slag}{Cement} \right) \right\}$ takes into

349 account the cement substitution by silica fume or slag, the prefactor C depends on the water-to-

350 cement and aggregate-to-cement ratios : $C = \frac{100}{(w/c)^{2.5} + \left(\frac{a/c}{10}\right)^{1.5}}$ and the exponent factor n , close to 0.2,

351 reads $n = 1.2 - 0.1(a/c) + (-0.14 + 0.005(a/c)) \ln C$.

352 • Modified B4 S model [73]:

353 The autogenous shrinkage value can be calculated using the 28d compressive strength

354 without any information regarding the formulation and reads:

$$\epsilon_{au}(t) = 12 f_c (1 - g)^{1.7} t^{0.2} \quad (20)$$

355 where f_c is the 28d compressive strength and $g = (\text{volume of aggregates}) /$

356 $(\text{volume of concrete})$ (default values of 0.7 and 0.0 can be used for concrete and cement pastes

357 respectively).

358 • CEB MC 10 model:

$$\epsilon_{cas}(t) = \epsilon_{cas0}(f_{cm}) \cdot \beta_{as}(t) \quad (21)$$

359 where $\beta_{as}(t) = 1 - \exp(-0.2\sqrt{t})$ the time function of autogenous shrinkage and

360 $\epsilon_{cas0}(f_{cm}) = -\alpha_{as} \left(\frac{0.1 f_{cm}}{6 + 0.1 f_{cm}} \right)^{2.5} \cdot 10^{-6}$ the notional autogenous shrinkage coefficient, where α_{as}

361 is a coefficient depending on cement type and f_{cm} is the 28-d compressive strength.

362 • CEB MC 10 modified for SCM consideration [15]:

$$\epsilon_{cas}(t) = k_{SCM} \cdot \epsilon_{cas0}(f_{cm}) \cdot \beta_{as}(t) \quad (22)$$

363 where k_{SCM} is a correction factor to included the impact of SCM which, in the case of

364 autogenous shrinkage, reads $k_{SCM} = (1 + 0.24f + 0.4m - 0.35s) \cdot 4M$ where f is the replacement

365 ratio of fly ash (%), m the replacement ratio of calcined clay (%), s the replacement ratio of slag

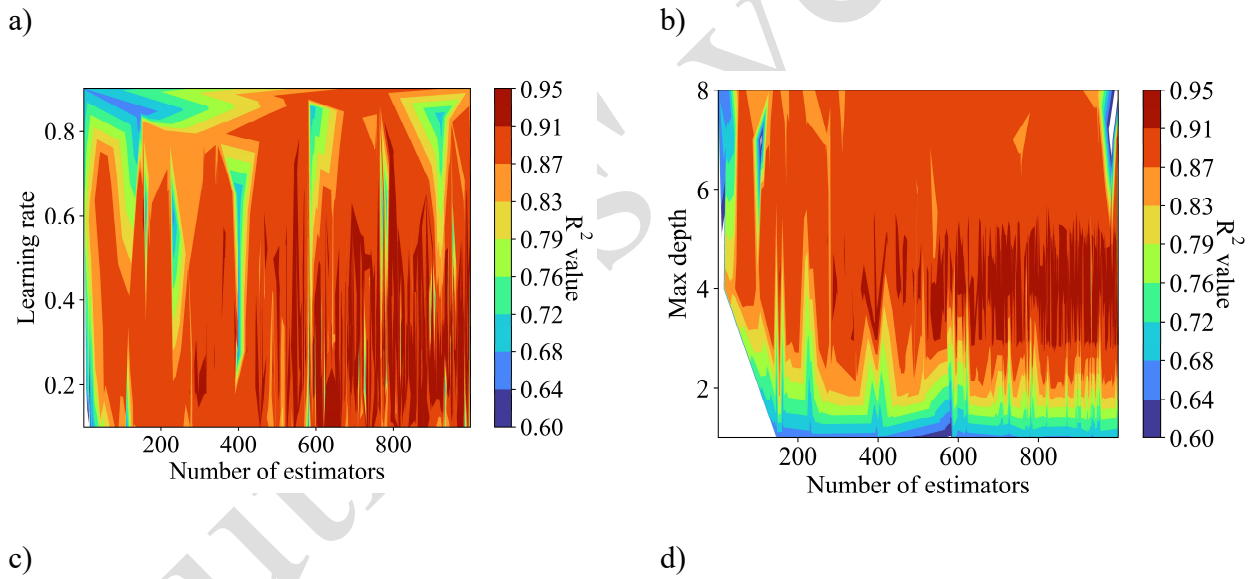
366 and M the multi-SCM coefficient (binary $M = 0.95$, single $M = 1.0$).

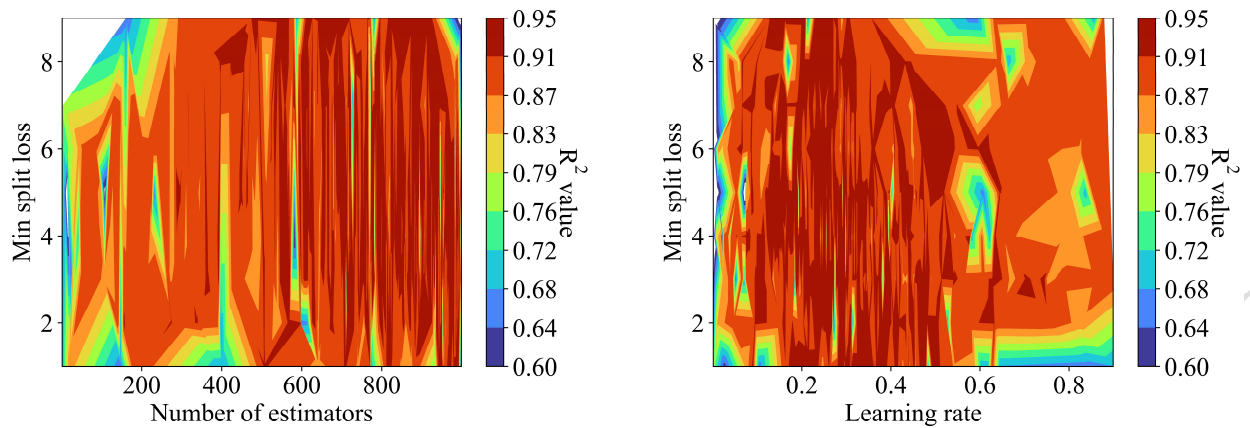
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368 **4 Results and Discussion**

369 **4.1 Models hyperparameters tuning**

370 The ML model parameters have been tuned using the Simulated Annealing (SA) optimization
371 to obtain the most performant model considering R^2 metric. Surface plots of the R^2 values for
372 several hyperparameter values of the XGB model are reported in Fig. 5. As illustrated in these
373 figures, extended zones of optimized parameter values could be found in most cases. For example,
374 as illustrated in Fig. 5 a), R^2 values higher than 0.91 could be obtained for learning rates lower than
375 0.5 and more than 500 iterations. A maximum depth of 4 led to the best results as illustrated in
376 Fig. 5 b) while various values of the minimum loss reduction required to make a partition on a leaf
377 node of the tree (min split loss) could generate good results, as illustrated in Fig. 5 c) and d). Based
378 on this optimization analysis carried out by SA, the best hyperparameters values of the four ML
379 models were selected. These values are reported in Table 2.





380 **Fig 5.** Tuning XGBoost hyperparameters: surface plots of R^2 -values using 10-fold cross-validation.

381

382 **Table 2.** Tunned hyperparameters of the ML models.

XGB	Nb of trees	Learning rate	Max depth	Min split loss			R^2
	1197	0.6680	10	4			0.9311
GB	Nb of trees	Learning rate	Max depth	Max features	Min samples split	Min samples leaf	R^2
	887	0.2740	10	10	0.0560	0.0580	0.9284
SVM	C	γ	ϵ	Kernel			R^2
	1491	0.3610	0.0610	RBF			0.8089
ANN	Nb of neurons	Activation	Solver	Max iteration			R^2
	(19,9)	RELU	LBFGS	4000			0.8054

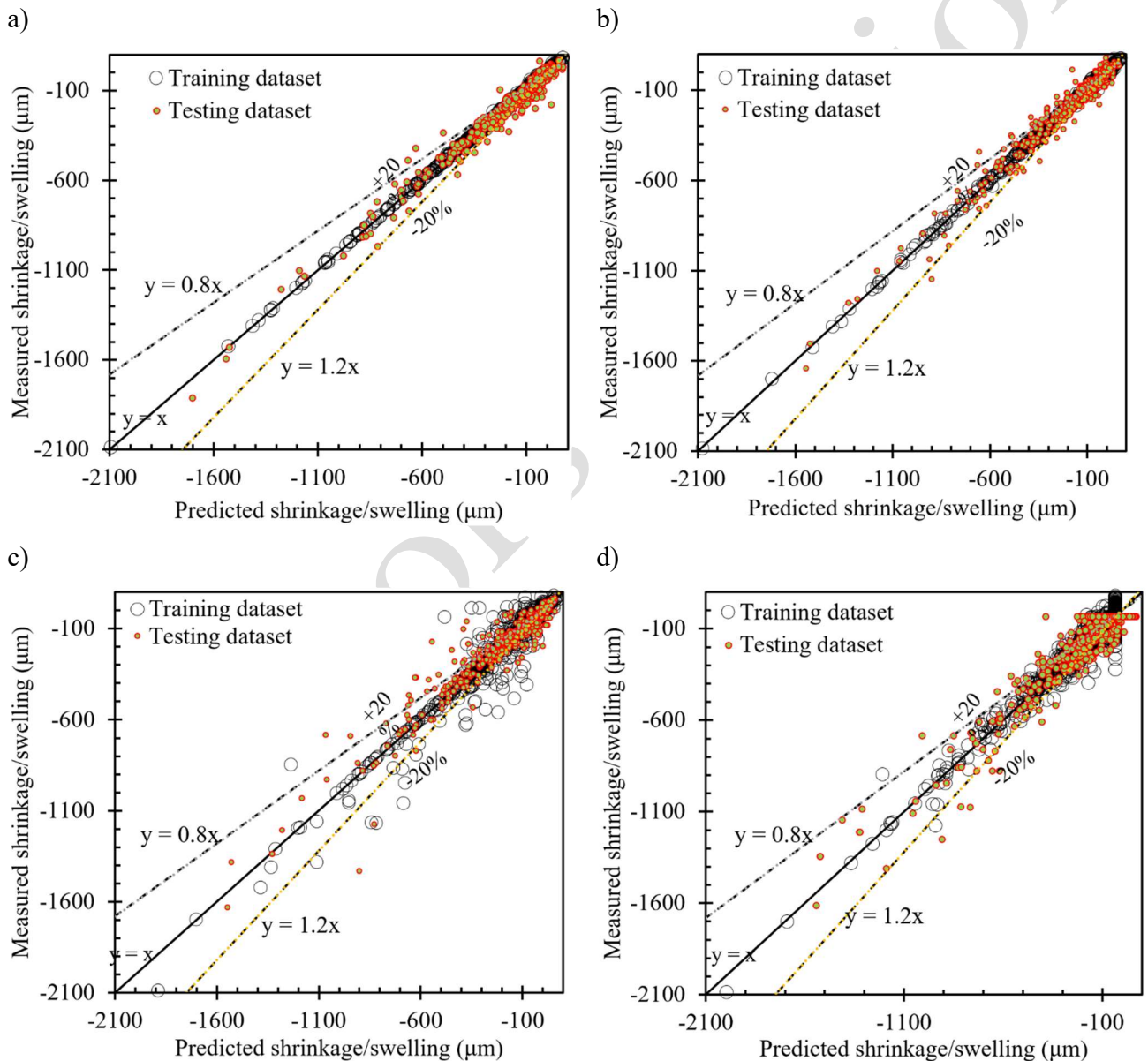
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384 4.2 Machine learning models typical predictions

385 The results obtained by the four models on the training and test sets are displayed in Fig. 6. As
 386 illustrated in the figure, all models performed well on the training sets with R^2 values higher than 0.94.
 387 Most training set predictions fall within the interval between 0.8 times and 1.2 times the measurement
 388 shrinkage value, except for very small shrinkage values. However, Gradient Boosting and XGBoost
 389 algorithms outperformed SVM and ANN models. The first two models provided high-quality predictions
 390 for various shrinkage values, while the latter two models were relatively prone to errors, even for small

391 shrinkage values. The detailed metrics corresponding to the model results are reported in Table 3. XGB
 392 model performed better than the other models, and the R^2 value associated with its prediction of the test
 393 set was 0.9733, which corresponds to an RMSE of around $38.9 \mu\text{e}$.

394 The mean absolute error (MAE) distribution has been analyzed for the four models, as illustrated in
 395 Fig. 7. It can be seen that the MAE remained limited for the XGB model as compared to the SVM and
 396 ANN models. Moreover, the maximum MAE measured for the XGB model, close to $200 \mu\text{e}$ was almost
 397 twice as small as the maximum MAE obtained by the SVM and the ANN model.

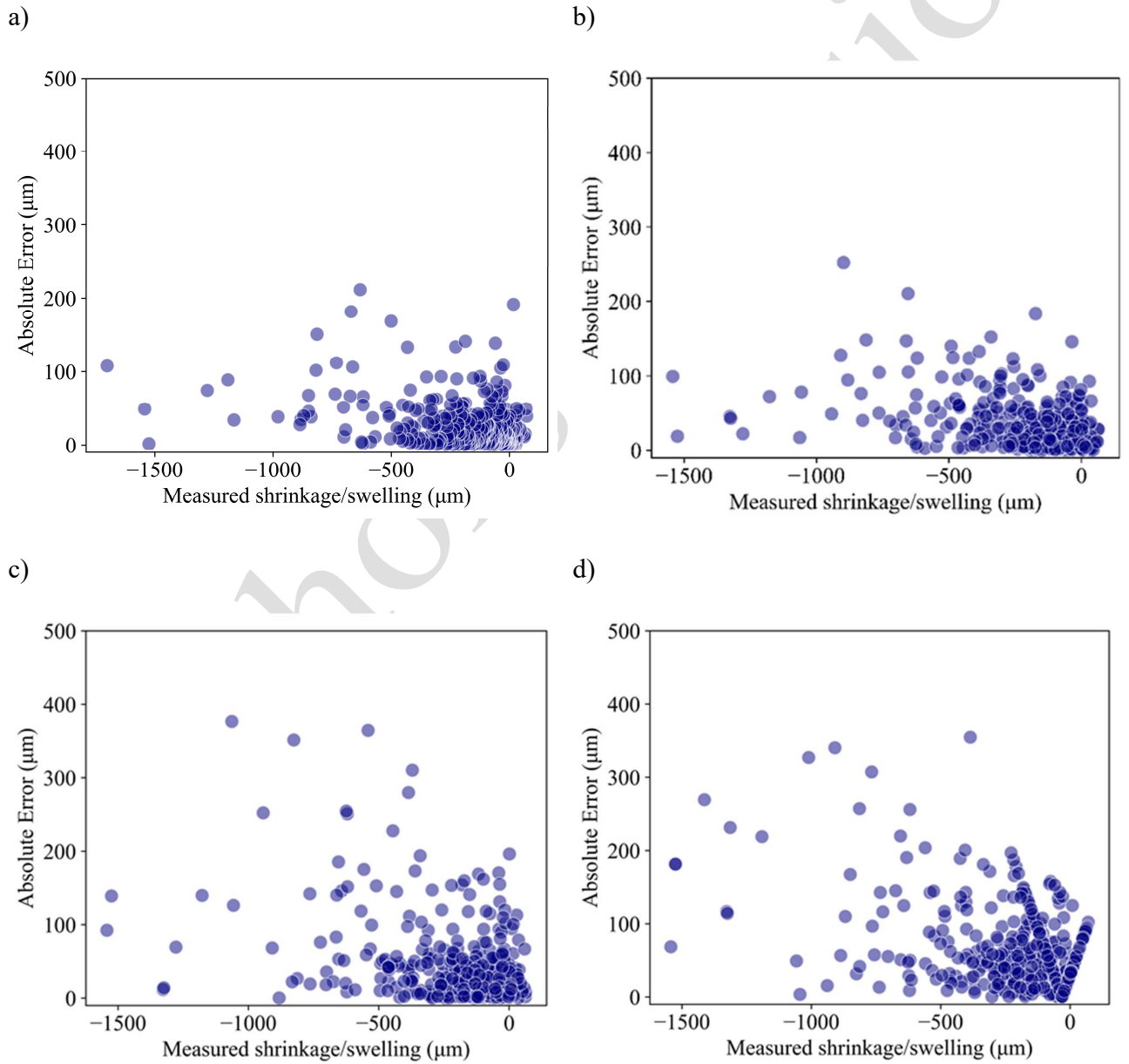


398 **Fig. 6.** Shrinkage/Swelling predicted by different ML models: a) XGB, b) GB, c) SVM and d) ANN
 399 models

400 **Table 3.** Comparison of machine learning algorithms for autogenous shrinkage prediction of
 401 concrete incorporating SCM.

	Train			Test		
	R ²	RMSE (μϵ)	MAE (μϵ)	R ²	RMSE (μϵ)	MAE (μϵ)
XGB	0.999	6.341	3.993	0.973	38.909	25.249
GB	0.998	7.816	4.620	0.965	45.797	31.039
SVM	0.941	57.085	21.974	0.915	71.775	40.764
ANN	0.949	50.695	37.303	0.910	79.288	56.594

402



403 **Fig 7.** Distribution of the absolute error: a) XGB, b) GB, c) SVM, and d) ANN models.

404 4.3 Feature importance and sensitivity analysis

405 4.3.1 Global interpretation

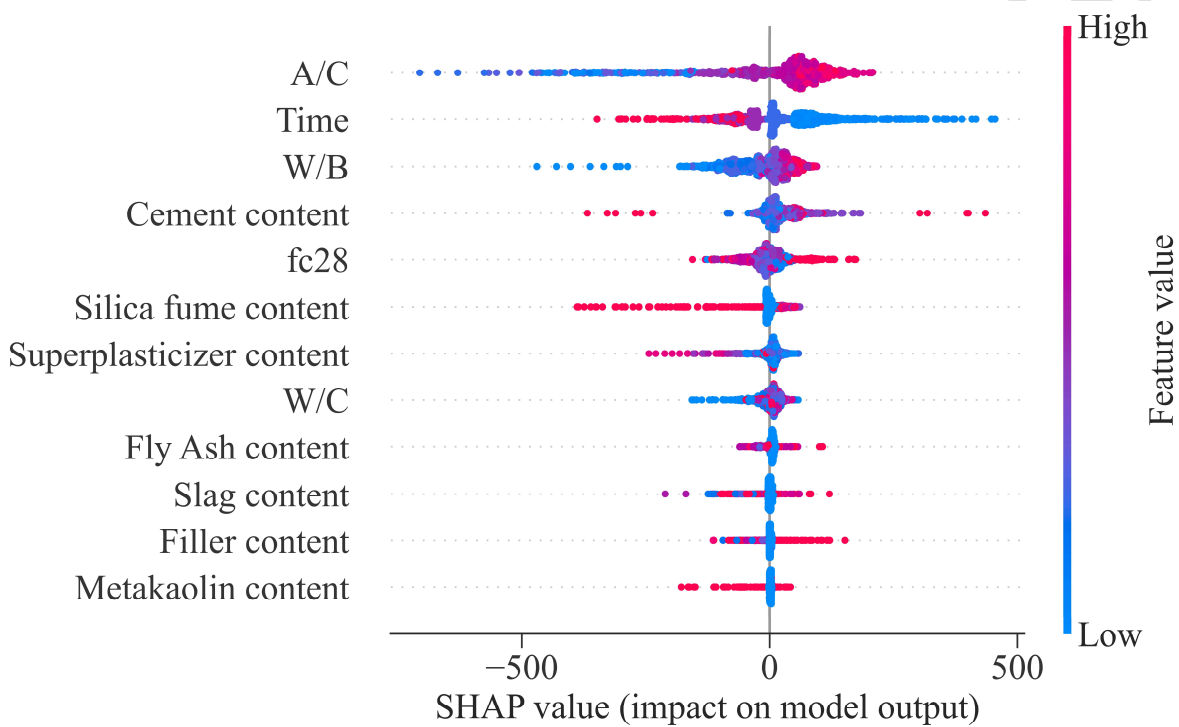
406 The most influential features on the shrinkage predictions have been obtained from the model
407 using SHAP. The global SHAP values are reported in Fig. 8, the features classified in descending
408 order based on their influence from top to bottom. The results align with the previous study
409 published by the authors dedicated to autogenous shrinkage prediction of cementitious materials
410 incorporating SAP and SCM even if the database has been largely extended and the model results
411 improved [44]. Indeed, the most influential parameters are the A/C ratio, time, W/B ratio, cement
412 content, the 28d compressive strength, silica fume content, superplasticizer content, W/C ratio, fly
413 ash, slag, filler, and last calcined clay content. The relative influence of the most influential
414 parameters can still be easily determined:

- 415 • increasing A/C ratio increases SHAP value, e.g., decrease shrinkage
- 416 • increasing time values correspond to higher shrinkage values
- 417 • increasing W/B and W/C ratios tend to decrease shrinkage
- 418 • high silica fume replacement ratio or cement content predominantly induces higher
419 shrinkage

420 However, the global influence of the other parameters, mainly SCM other than silica fume,
421 might not be that clear at first sight. Most fly ash highest values are associated with positive SHAP
422 values, which means that a high fly ash content globally decreases shrinkage. Similarly, the highest
423 filler contents are associated with positive SHAP values, i.e., decreased shrinkage. Since the
424 highest calcined clay contents are associated with the most negative SHAP values, its adverse
425 effect on autogenous shrinkage can be confirmed for high replacement ratios. Last, slag and 28d
426 compressive strength effects cannot be analyzed easily from this global perspective. To this end,
427 more detailed insights are needed using the features dependence plots.

428 SHAP can also give information about the feature dependency of the results, as illustrated in
429 Fig. 9. Indeed, feature dependence plots reveal how the SHAP values change depending on the
430 values of the features. As illustrated in Fig. 9 a), the SHAP values largely increase when the A/C
431 values increase, especially when A/C values increase from around 1.0 to 4.0, corresponding to the
432 transition from mortar to concrete. This increase of around $800 \mu\epsilon$ highlights the relative influence

433 of the A/C ratio on the autogenous shrinkage phenomenon. For A/C values higher than 4.0, SHAP
 434 value is almost constant, meaning there is no interest in further increasing the A/C ratio to reduce
 435 the autogenous shrinkage. The water-to-binder ratio's influence can be analyzed using Fig. 9 b).
 436 From this figure, it can be seen that the SHAP value increases from the minimum w/b considered
 437 in this study, e.g. 0.16, to approximately 0.5. This gradual increase from around $-300 \mu\epsilon$ to around
 438 $50 \mu\epsilon$ confirms that autogenous shrinkage arises in cementitious materials of W/B ratio smaller
 439 than 0.5. However, it is worth noting that the W/B relative influence is around twice as small as
 440 the A/C influence.



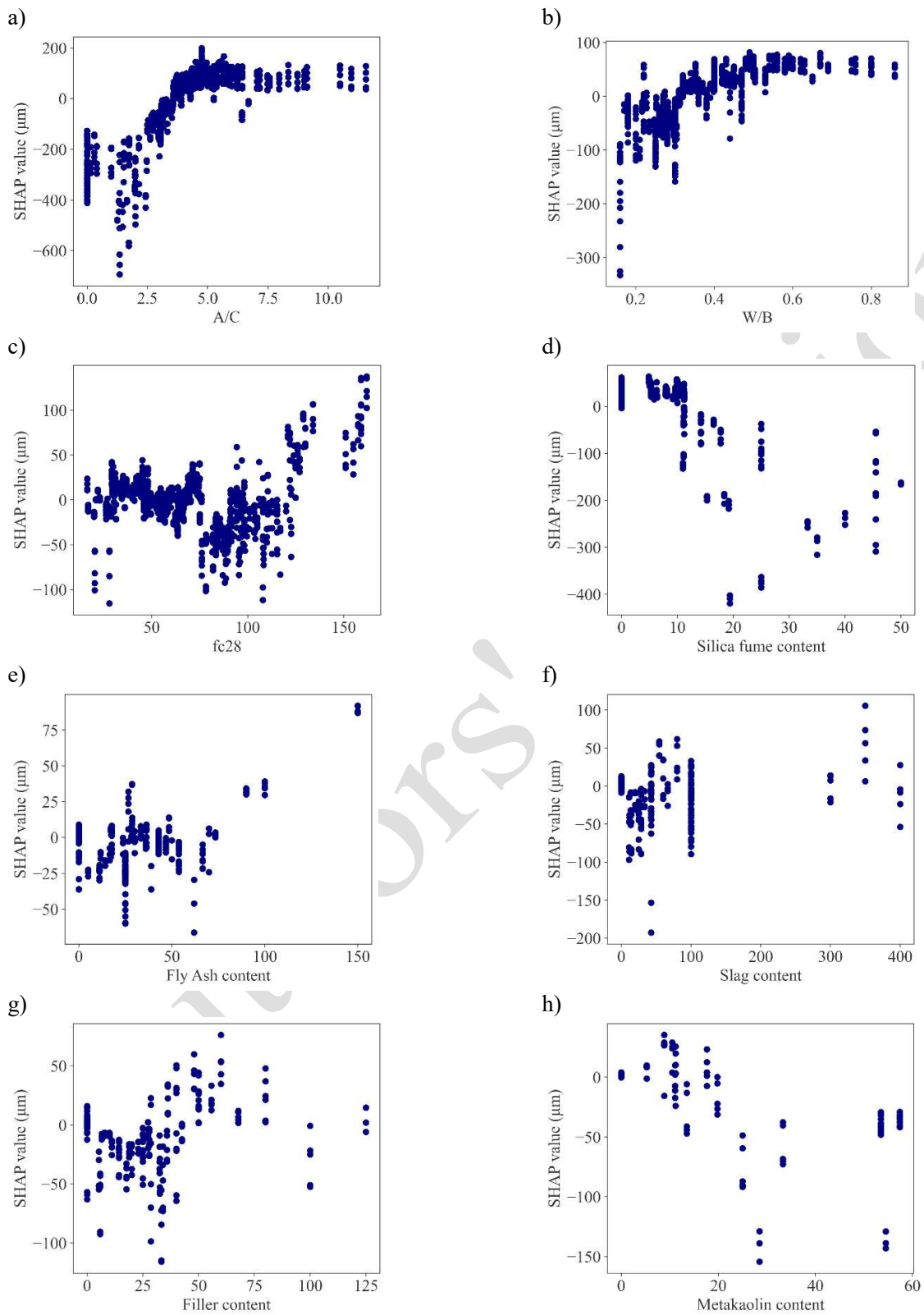
441
 442 **Fig. 8.** Global SHAP values of the tuned XGB model

443 Based on Fig. 9 c), it can be seen that the increasing strength values up to around 100MPa
 444 negatively influence SHAP values, which means that transitioning from normal strength to high
 445 strength concrete leads to more autogenous shrinkage, independently from the other parameters
 446 such as the W/B ratio. Conversely, SHAP values increase for strength higher than around 100MPa
 447 up to final values around $140 \mu\epsilon$, which means that autogenous shrinkage for this type of high
 448 performance and ultra-high performance concrete would have been more pronounced if their
 449 strength had been smaller. This novel insight might correlate to the quick strength and Young's
 450 modulus increase of these concretes, limiting early age autogenous shrinkage.

451 The influence of silica fume can be analyzed using Fig. 9 d). Based on this figure, it can be
452 observed that increasing silica fume values, from 0% to 50% cement replacement, largely
453 decreases SHAP values. However, a spread should be noticed when the silica fume replacement
454 ratio is larger than 20%, and it should be noticed that a 50% replacement ratio can influence SHAP
455 values less than a 20% replacement ratio in the case of some concretes. Therefore, although silica
456 fume is known to increase considerably autogenous shrinkage, novel routes might be found to limit
457 its influence. The other supplementary cementitious materials have a smaller influence on SHAP
458 values. As illustrated in Fig. 9 e), fly ash influence on SHAP values becomes visible on this feature
459 dependence plot for replacement ratios higher than 50%. In this case, cement substitution by fly
460 ash leads to smaller autogenous shrinkage values explained by the slower hydration. Based on Fig.
461 9 f), it can be observed that slag influence on SHAP values is relatively limited as most of the
462 values belong to the $[-100 \mu\epsilon, 50 \mu\epsilon]$ interval. However, it is worth noting that, according to this
463 detailed analysis, slag negatively influences shrinkage for all the substitution ratios smaller than
464 around 50%, which agrees with the literature [19,74]. On the opposite, different behaviors can be
465 observed for replacement ratios higher than 50%: slag can positively affect shrinkage sometimes,
466 while it still negatively influences shrinkage for other concrete mixes. It can be hypothesized that
467 two competing interests are at stake: the refined pore structures that increase shrinkage and the
468 slower hydration that decrease shrinkage at a given time. As illustrated in Fig. 9 g), filler globally
469 slightly increases shrinkage for substitution rates smaller than 25%, which can be explained by the
470 increased hydration speed. However, substitution ratios higher than 25% systematically positively
471 influence SHAP values, highlighting the restraining effect of filler on the autogenous shrinkage.

472 Finally, though the effect of calcined clay is relatively small according to the model, it can be
473 observed that calcined clay does not influence SHAP values a lot for replacement ratios smaller
474 than 20%, while increasing the substitution rate, the SHAP values decrease. This observation
475 agrees with the literature [24,58]. To conclude, since SHAP gives the influence rules of the
476 different features on the autogenous shrinkage predictions of the model, it can be used to provide
477 novel insights into the shrinkage phenomenon.

478



479 **Fig. 9.** Feature dependence plots associated with SHAP for the influential features: a) A/C, b)
 480 W/B, c) fc28, d) silica fume, e) fly ash, f) slag, g) filler, and h) calcined clay.

481 4.3.2 Local interpretation

482 Besides global interpretations, SHAP also provides useful information to explain the model
483 predictions on individual samples as SHAP decomposes the final prediction into a sum of
484 contributions by all the input variables. Various 28d autogenous shrinkage predictions were thus
485 analyzed for several unknown concrete samples containing various types of SCM. Fig. 10
486 illustrates explanations for four typical samples.

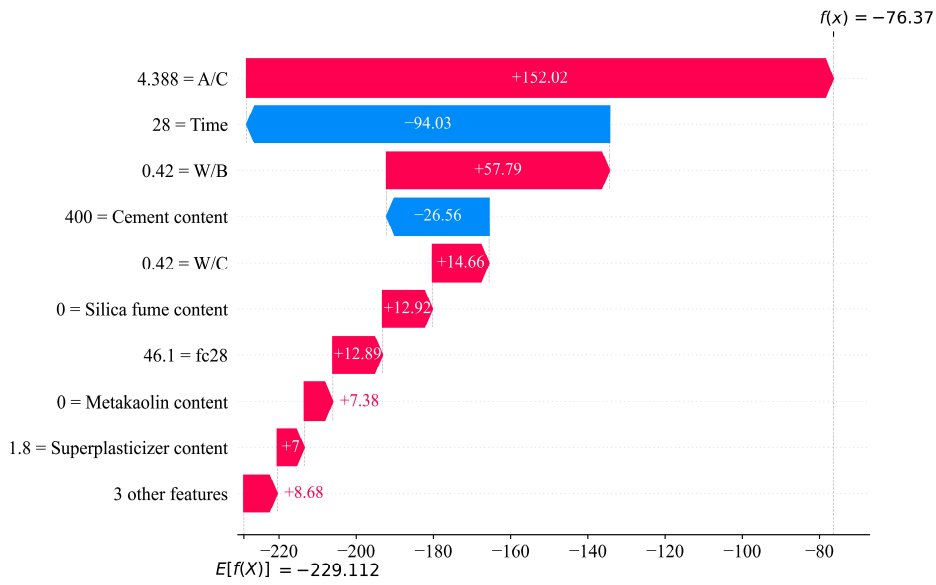
487 As shown in Fig. 10 a), the base prediction on the entire set is $-229 \mu\epsilon$. For this sample, the
488 most significant reason for the final autogenous shrinkage prediction of $-76 \mu\epsilon$ is the A/C ratio,
489 whose individual contribution amounts to $+152 \mu\epsilon$, meaning this value decreases shrinkage
490 compared to lower A/C ratios. Then time negatively influences the autogenous shrinkage
491 prediction, which can be explained by the fact that 28 days is the final prediction associated with
492 larger shrinkage deformations. The water to binder ratio is the third most influential parameter, as
493 expected based on the global interpretation.

494 For concrete incorporating silica fume, its relative influence on the outputs can be quantified
495 as illustrated in Fig. 10 b). The presence of silica fume can considerably influence the model
496 prediction. Indeed, as illustrated in the figure, silica fume content becomes the most influential
497 parameter, and, at 28 days, the SHAP value associated to silica fume is around $-160 \mu\epsilon$.

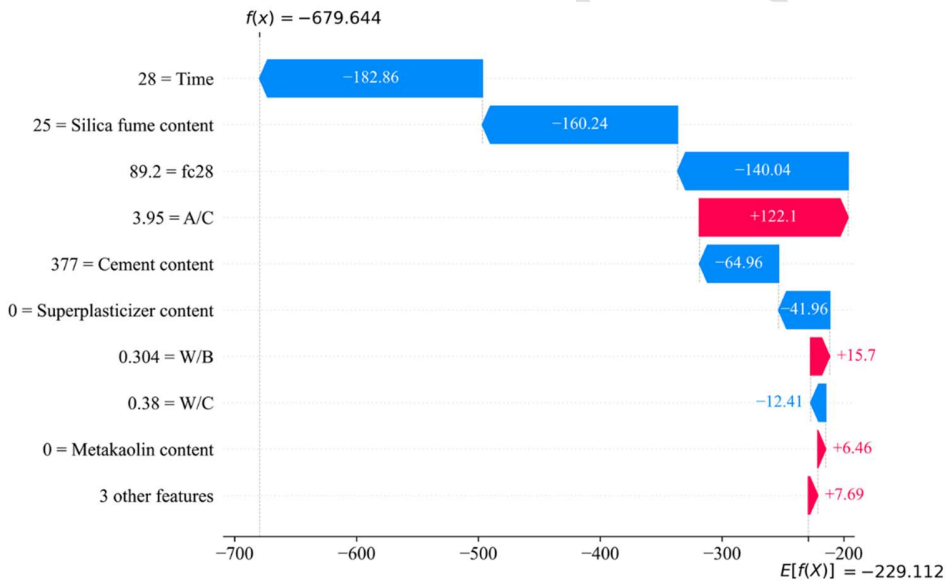
498 In most analyses, small replacement ratios of other SCM were found only slightly to affect
499 shrinkage values as the A/C and the W/B ratios predominantly influenced the latter, as illustrated
500 in Fig. 10 c) represents the inputs contributions on the autogenous shrinkage prediction of a
501 concrete sample incorporating fly ash with the mass of fly ash equal to 11.1% of the one of cement.
502 However, when larger proportions of cement are replaced, the influence of the SCM can become
503 predominant. Indeed, as illustrated in Fig. 10 d), when half of the cement is replaced by slag, this
504 slag proportion increases shrinkage by around $52 \mu\epsilon$ according to the model.

505

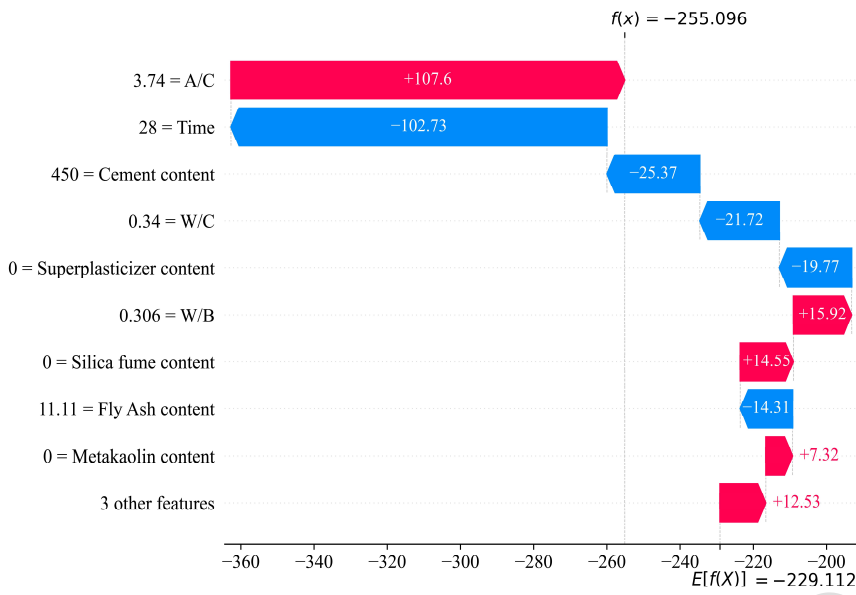
a)



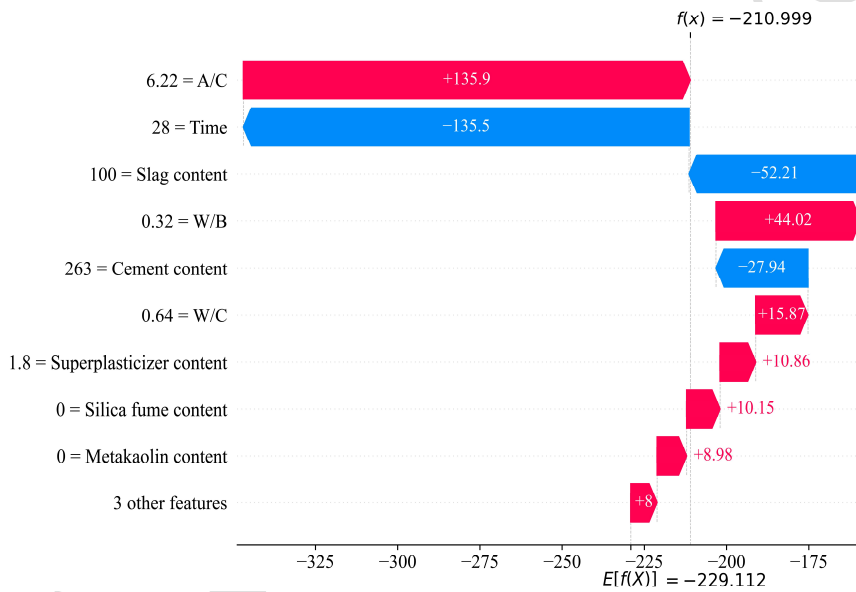
b)



c)



d)



506 **Fig. 10.** Local interpretation using SHAP of some of the XGB model autogenous shrinkage
 507 predictions: a) normal strength concrete without SCM, b) high strength concrete with silica fume,
 508 c) normal strength concrete with fly ash, d) high-strength concrete with 50% of cement replaced
 509 by slag.

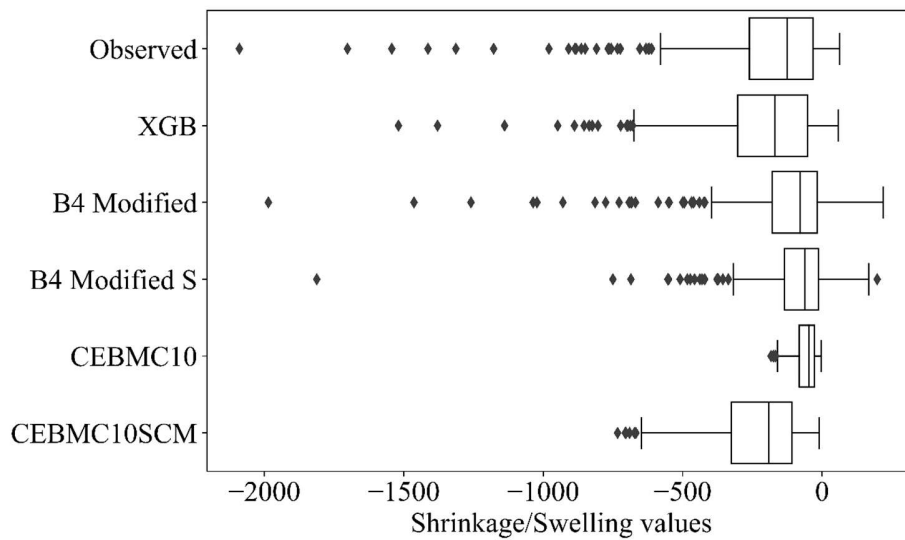
510

511 4.4 Comparison with B4 and CEB analytical models

512 The developed XGBoost model, the modified B4 and B4s, the CEB MC10, and the CEB MC

513 10 model's modified version can be compared globally using their respective predictions on the
514 test set composed of unknown concrete formulations. The performance of these four models has
515 been compared with the observed shrinkage values, as illustrated in Fig. 11. It can be observed
516 that, overall, the distribution of the shrinkage values predicted by the developed XGB model is in
517 close agreement with the observed distribution, and the box plots are very similar. Indeed,
518 interquantiles ranges and outliers present similar patterns. The XGB model slightly overestimates
519 the overall shrinkage values, which is good regarding safety issues. Last but not least, the XGB
520 model can predict small swelling values that might occur at an early age, while analytical models
521 cannot be captured correctly this trend.

522 The analytical models' performance considerably varies. Based on the overall distribution of
523 the shrinkage values, the modified B4 model provides a distribution of the predictions that is in
524 good agreement with the observed distribution. However, one can observe that the mean shrinkage
525 value predicted by the modified B4 model slightly underestimates the observed shrinkage
526 distribution, which might represent a risk regarding safety. The same conclusion applies to the
527 modified version of the B4 S model. Moreover, the predictions made by this model cannot capture
528 the experimental variability, probably due to its simplicity. CEB MC 10 model results clearly
529 underestimate shrinkage, and the size of the overall distribution is considerably smaller than the
530 observed distribution, highlighting the shortcomings of this analytical model. The modified
531 version of the CEB MC 10 model performed better, and the overall distribution of the shrinkage
532 values looks like the observed distribution as the interquartile range is close to the experimental
533 one. However, an apparent overestimation of the shrinkage values and a disability to predict large
534 shrinkage values can be noticed.



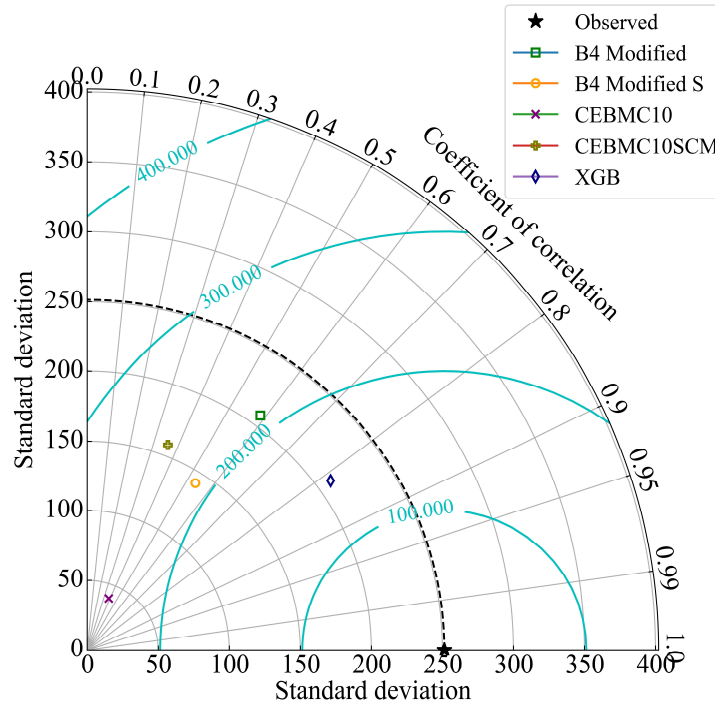
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536 **Fig. 11.** Box plots of the shrinkage/swelling values predicted by the XGB model compared to
 537 the analytical models and the observed values

538

539 The model results and the test data can be further compared using the Taylor diagram (Fig.
 540 12), which summarizes three valuable characteristics of the models compared to the measured
 541 values: the standard deviation associated with the model's predictions, the correlation between the
 542 predictions and the experimental values, and the centered root-mean-square (RMS) difference. As
 543 mentioned in the previous paragraph, the standard deviation of the simulated patterns reported on
 544 the X-axis largely differs between the models. The standard deviation of the experimental data is
 545 almost reproduced by the XGB and the modified version of the B4 model. Indeed, the standard
 546 deviations associated with these models are higher than $200 \mu\epsilon$, close to the $250 \mu\epsilon$ experimental
 547 value. Then, the modified B4 S and modified version of the CEB MC 10 model exhibit a standard
 548 deviation of around $150 \mu\epsilon$, which is in relatively good agreement with the observed values. Last,
 549 the standard deviation of the classic CEB Model 10 is smaller than $40 \mu\epsilon$, clearly underestimating
 550 the experimental variation and highlighting the model's shortcomings in predicting shrinkage of
 551 concrete incorporating SCM. Concerning the correlation of the models with the experimental
 552 values, the best correlation is obtained by the XGB model (0.82). This correlation is largely higher
 553 than the second-best correlation obtained by the modified B4 model (0.58). The correlation of the
 554 modified B4 S model follows. The CEB MC 10 and the modified version of the CEB MC 10 model
 555 exhibit correlations close to 0.3-0.4, which is relatively small. Finally, the RMS value of the XGB

556 model (around $160 \mu\epsilon$) is clearly better than the ones of the other models, which are higher than
 557 $200 \mu\epsilon$. For all these reasons, it can be concluded that the optimized XGB model significantly
 558 outperforms the best analytical models that have been proposed up to date.



559
 560 **Fig. 12.** Taylor diagram representing XGB, B4 and B4s modified, CEB MC 10 and CEB MC
 561 10 modified version models performance.

562
 563
 564 Based on the XGB model, the autogenous shrinkage predictions of the eight concrete
 565 compositions containing various types of SCM have been compared to the analytical models'
 566 predictions, as shown in Fig. 13. The detailed formulations are given in Table 4. As illustrated in
 567 these figures, the prediction accuracy of the XGB model globally outperforms that of the analytical
 568 models in most cases which agrees with Taylor's analysis.

569
 570
 571
 572
 573

574 **Table 4.** Mortar and concrete compositions of some typical test samples.

Ref	C1	C2	C3	C4	C5	C6	C7	C8
W/C	0.42	0.38	0.34	0.64	0.29	0.43	0.31	0.44
W/B	0.42	0.304	0.306	0.32	0.28	0.3	0.21	0.3
A/C	4.39	3.95	3.74	6.22	4.21	3.68	3.94	3.74
Cement (kg/m ³)	400	377	450	263	428	408	497	416
Silica fume (%)	-	25	-	-	-	14.2	10	-
Fly Ash (%)	-	-	11.1	-	-	28.7	-	-
Slag (%)	-	-	-	100	-	-	-	-
Metakaolin (%)	-	-	-	-	5.3	-	-	10.5
Filler (%)	-	-	-	-	-	-	34	36.2
Sp (%)	1.8	-	-	1.8	3.1	2.1	2.07	1.46
fc28 (MPa)	46.1	89.2	53.4	66.7	91.5	69.7	93	84
Time (days)	1-28	1-28	1-28	1-28	1-28	1-28	1-28	1-28

575

576 In the case of a normal strength concrete with a water-to-binder ratio of 0.42 and without any
 577 SCM, the model's prediction agrees with the experimental values, and only a 20 $\mu\epsilon$ difference is
 578 obtained after 28 days, as illustrated in Fig. 13 a). However, the B4 model better predicted the
 579 long-term 28-d shrinkage value. The CEB MC 10 model's modified version largely overestimated
 580 the autogenous shrinkage values. On the opposite, as observed in the global statistics, the CEB
 581 MC 10 model underestimates the autogenous shrinkage at 28 days.

582 The effect of the cement substitution by silica fume is illustrated in Fig. 13 b). Both the XGB
 583 model and the modified version of the CEB MC 10 model can provide good predictions, while the
 584 modified versions of the B4 model largely underestimate autogenous shrinkage by around 300 $\mu\epsilon$
 585 and the CEB MC 10 model underestimates the shrinkage value by approximately 400 $\mu\epsilon$.

586 As illustrated in Fig. 13 c), the XGB model prediction of the shrinkage values of concrete with
 587 a relatively low W/B around 0.3 incorporating fly ash closely matches the experimental values,
 588 even at an early age. The analytical models' predictions are relatively far from the experimental
 589 values at an early age, which might be attributed to these models' absent or relatively recent
 590 considerations of fly ash effects. It should be noticed that the 28d shrinkage values predicted by
 591 the modified versions of the B4 and CEB MC10 model are in relatively good agreement with the
 592 experimental values, but their prediction might deviate from the measured values for more
 593 extended periods.

594 Fig. 13 d) displays the autogenous shrinkage predictions of the models in the case of high-

595 strength concrete, with a water-to-binder ratio of 0.32, in which 50% of cement has been replaced
596 by slag. In this case, exemplifying modern concretes with high substitution rates, the XGB model
597 also performed well, though slightly underestimating the 28d autogenous shrinkage value. The
598 modified B4 model provides the best prediction, but the modified version of the B4 S model
599 underestimated the shrinkage values as well. The CEB MC 10 models underestimated the
600 shrinkage values, while the modified version of the CEB MC 10 whose prediction can be qualified
601 as correct, still overestimated the shrinkage value by around $75 \mu\epsilon$. It would be interesting to
602 combine analytical and machine learning models in such a case.

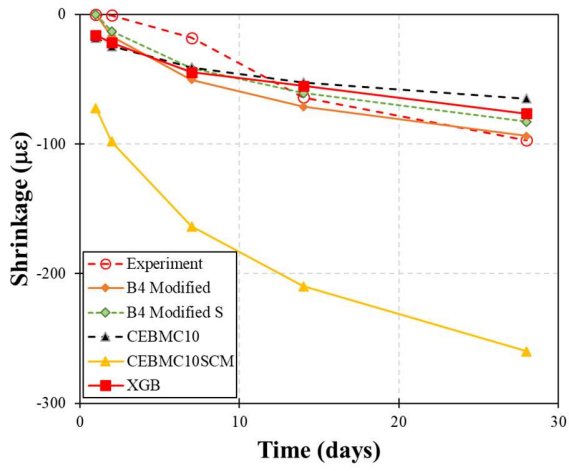
603 Though more experimental data is needed regarding the influence of calcined clay on drying
604 and autogenous shrinkage, the developed XGB model showed better results than the analytical
605 models in predicting the autogenous shrinkage evolution of concrete mixes incorporating calcined
606 clay, as illustrated in Fig. 13 e). The analytical models which do not consider the effect of calcined
607 clay - modified B4, modified B4 S and CEB MC 10 models - largely underestimated the shrinkage
608 values, while the modified version of the CEB MC 10 models overestimated its influence.

609 The prediction quality of the models can also be calculated in the case of ternary cement
610 blends. As illustrated in Fig. 13 f), the XGB model captured the combined effect of silica fume
611 and fly ash satisfactorily, as the 28d autogenous shrinkage prediction differs by around $60 \mu\epsilon$ from
612 the experimental value, but overestimates early age shrinkage. In this case, the modified version
613 of the B4 model outputs good yet slightly underestimated results. However, the prediction of the
614 autogenous shrinkage of some ternary formulations might be improved in the future. As illustrated
615 in concrete in Fig. 13 g), the XGB and analytical models predictions are pretty far from the
616 measured values for concrete in which cement is partially substituted by silica fume and filler. In
617 this particular case, the modified version of the CEB MC 10 model provided the best estimation
618 of the final 28-day shrinkage value.

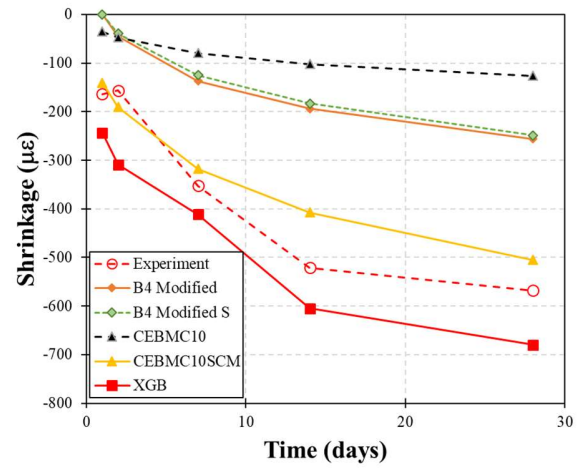
619 The XGB model's predictions are better in the case of LC³ concrete incorporating calcined
620 clay and filler, as illustrated in Fig. 13 h) since several formulations of this type are present in the
621 database. In that case, the model predictions are good, especially after 10 days, while the early
622 shrinkage values are overestimated. Other models cannot capture the experimental shrinkage
623 evolution.

624

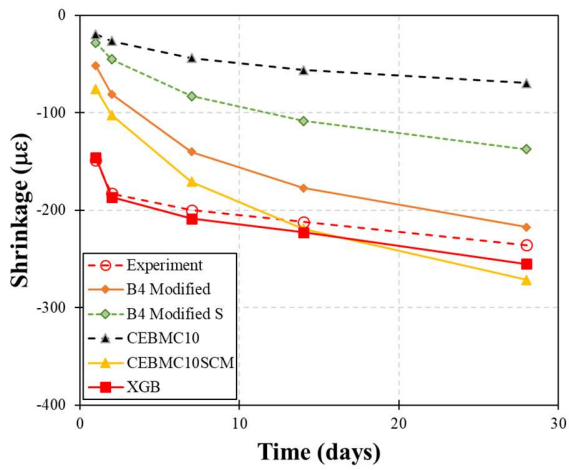
a)



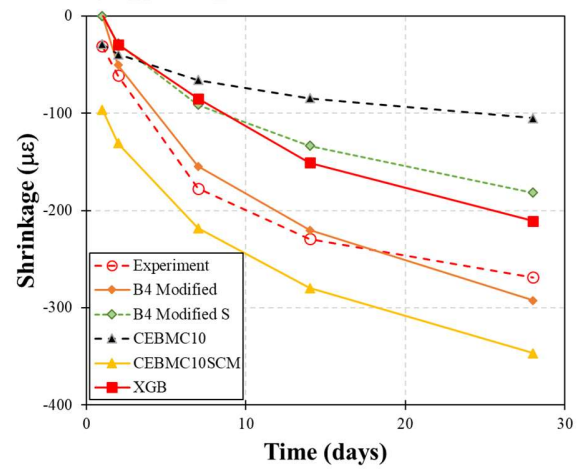
b)



c)

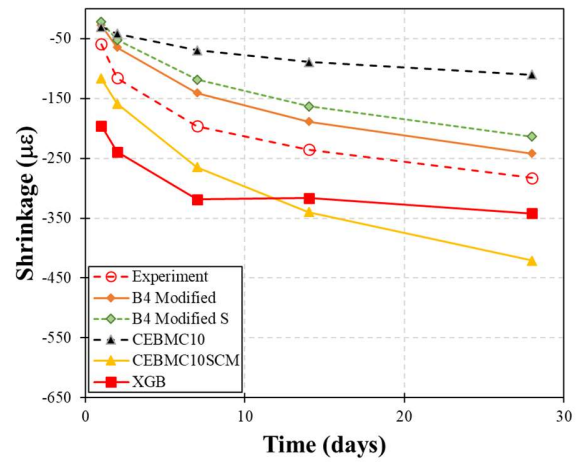
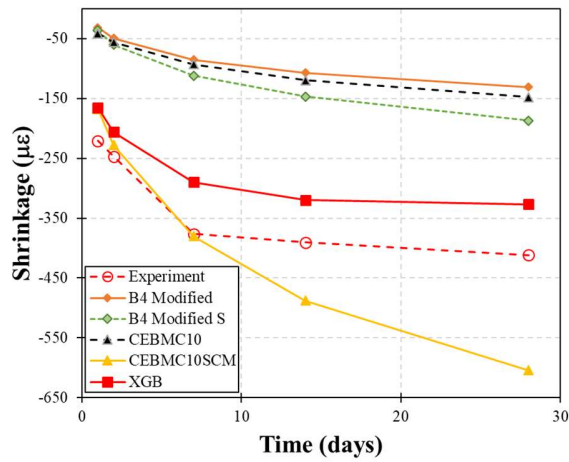


d)

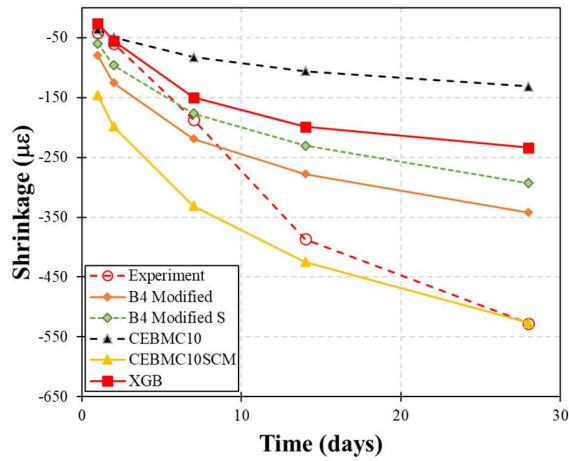


e)

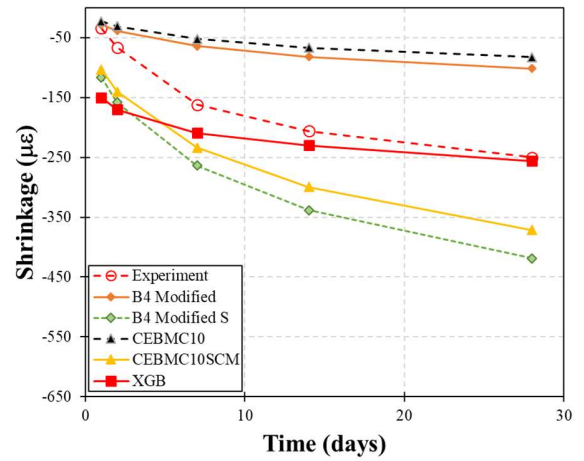
f)



g)



h)



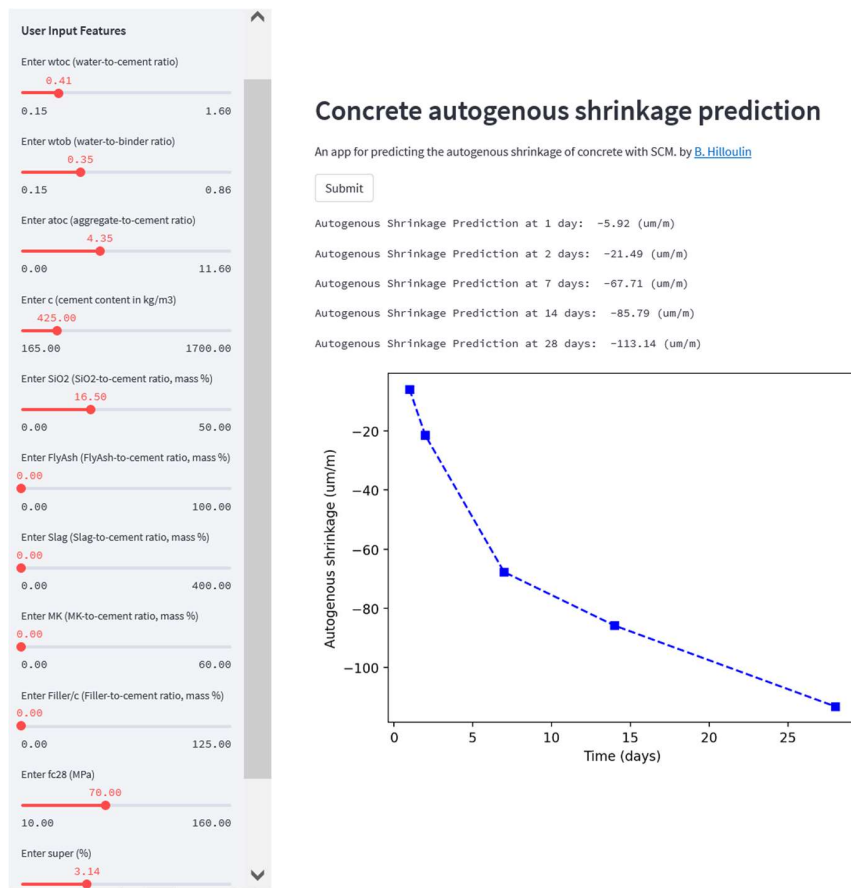
625 **Fig. 13.** Comparison of the autogenous shrinkage predictions of the XGB model and the
 626 analytical models for several unknown concrete formulations detailed in Table 4: a) normal
 627 strength concrete without SCM, b) high strength concrete with silica fume, c) normal strength
 628 concrete with fly ash, d) high-strength concrete with 50% of cement replaced by slag, e) high-
 629 strength concrete incorporating calcined clay, f) high-strength concrete with cement replaced by
 630 silica fume and fly ash, g) high-strength concrete with silica fume and filler, h) normal strength
 631 concrete incorporating calcined clay and filler (LC³ concrete).

632

633 4.5 Web application

634 A web application has been built using the first model trained on the whole database to provide
 635 autogenous shrinkage predictions of various concrete formulations. The user can input the concrete

636 formulation using several sliders whose minimum and maximum values corresponds to the ones
 637 from the database, and then predictions of the shrinkage values at 1 day, 2 days, 7 days, 14 days
 638 and 28 days are computed online based on the model developed in this study. Default values
 639 corresponding to a high-strength concrete formulation incorporating silica fume are considered
 640 from a study not included in the database [75]. A graph is plotted to visualize the predictions as
 641 illustrated in Fig.14. The web application is available at [https://share.streamlit.io/bhilloul/concrete-](https://share.streamlit.io/bhilloul/concrete-auto-shrinkage-ai-streamlit/main)
 642 [auto-shrinkage-ai-streamlit/main](https://share.streamlit.io/bhilloul/concrete-auto-shrinkage-ai-streamlit/main) .



643
 644 **Fig. 14.** Web application for autogenous shrinkage prediction of concrete incorporating SCM.

645
 646 **5 Conclusions**

647 This study examined the usage and potential of several Machine Learning (ML) algorithms to
 648 precisely predict the autogenous shrinkage of low-carbon cementitious materials with various
 649 types of supplementary cementitious materials (SCM) and compared the results with analytical
 650 models, e.g., the modified version of the B4 and B4 S models, the CEB MC 10, and the CEB MC

651 10 modified version. To this end, an extensive database of autogenous shrinkage measurements
652 has been built based on a previous study. First, Gradient Boosting (GB), XG Boost (XGB), Support
653 Vector Machine (SVM), and an Artificial Neural Network (ANN) model have been optimized
654 using grid search hyperparameter optimization, and their performance has been assessed using k-
655 fold cross-validation. The best model has been further analyzed using the Shapley Additives
656 Explanations (SHAP) to facilitate interpretations and provide novel insights into the autogenous
657 shrinkage mechanism. Finally, the developed model has been compared to the aforementioned
658 analytical models, some recently adapted to consider the effect of SCM. Based on the results, the
659 following main conclusions can be drawn:

- 660 • An extensive database composed of 1482 autogenous shrinkage curves of various
661 binary, ternary and quaternary cement paste, mortar, and concrete incorporating silica
662 fume, fly ash, slag, calcined clay, and filler, containing also concrete 28-day
663 compressive strength, has been built using data from the literature.
- 664 • ML models can accurately predict the autogenous shrinkage, and their
665 hyperparameters can be optimized through grid search. Indeed, R^2 values of around
666 0.805 to 0.931 have been obtained on the test set. The best model identified in this
667 study is XGB.
- 668 • The relative influence of the model inputs on the predictions can be analyzed using
669 SHAP values. Global SHAP values agreed with the experimental observations, and
670 the A/C ratio, time, W/B ratio, and silica fume content are particularly impacting.
671 Local SHAP analysis helped identify some evolutions of the shrinkage behavior with
672 increasing amounts of SCM, for example, the competition between the shrinkage
673 increase due to the pore refinement and the shrinkage delay due to slower hydration.
- 674 • The model predictions of completely unknown shrinkage behavior of concretes
675 incorporating SCM are significantly better than the predictions of analytical models
676 such as the modified B4 models, the CEB MC 10, and the modified version CEB MC
677 10, even though some analytical models can perform better predictions for specific
678 formulations. Detailed comparisons of the models' shrinkage predictions of various
679 concrete compositions have been studied thoroughly.
- 680 • A web application has been developed to provide fast and precise predictions to the

681 scientific and industrial community and drive further low-carbon cementitious
682 materials developments.

683 The study might open up novel research and industrial perspectives on shrinkage prediction
684 of eco-friendly cementitious materials using advanced Machine Learning techniques.

685 **CRedit authorship contribution statement**

686 **Benoit Hilloulin:** Conceptualization, Methodology, Investigation, Software, Formal analysis, Writing -
687 original draft, Writing - review & editing, Validation.

688 **Van Quan Tran:** Conceptualization, Methodology, Software, Visualization. Writing -original draft,
689 Writing - review & editing.

690

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

692

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695

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