

Soft Computing and Multi-Scal Model Technics to Predict the Early Age Compression Strength of Cement Paste as a Function of Polymer Contents, Water-to-Cement-Ratio, and Curing Ages

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1 **Soft Computing and Multi-Scal Model Technics to Predict the Early Age Compression**
2 **Strength of Cement Paste as a Function of Polymer Contents, Water-to-Cement-Ratio, and**
3 **Curing Ages**

4
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18
19
20 **Abstract**

21 In this study, the effect of two water reducer polymers with smooth and rough surfaces on the
22 compression strength of Ordinary Portland cement (OPC) was investigated. Three different
23 initial ratios between water and cement (w/c) 0.5, 0.6, and 1 were used in this study. The amount
24 of polymer contents varied from 0 to 0.06 % (%wt) for the cement paste with initial w/c of 0.5
25 and the polymer contents ranged between 0 to 0.16% (%wt) for the cement paste with initial w/c
26 of 0.6 and 1 were investigated. SEM test was conducted to identify the impact of polymers on
27 the behavior of cement paste. The compression strength of OPC cement was increased
28 significantly with increasing the polymer contents. Because of a fiber net (netting) around
29 cement paste particle was developed when the polymers were added to the cement paste which
30 leads to decrease the void between the particles, binding the cement particles, therefore,
31 increased the viscosity and compression strength of the cement rapidly. In this analysis, the
32 hardness of cement paste with polymer contents has been evaluated and modeled using four
33 different model technics. More environmentally sustainable construction, and lower cost than

34 conventional building materials and early age strengths of the cement. To overcome the
35 mentioned matter, this study aims to establish systematic multiscale models to predict the
36 compression strength of cement paste containing polymers and to be used by the construction
37 industry with no theoretical restrictions. For that purpose, a wide data a total of 280 tested
38 cement paste modified with polymers, has been conducted, analyzed, and modeled. Linear,
39 Nonlinear regression, M5P-tree, and Artificial Neural Network (ANN) technical approaches
40 were used for the qualifications. In the modeling process, the most relevant parameters affecting
41 the strength of cement paste, i.e. polymer incorporation ratio (0-0.16% of cement's mass), water-
42 to-cement ratio (0.5-1), and curing ages (1 to 28 days). According to the correlation coefficient
43 (R), mean absolute error and the root means a square error, the compression strength of cement
44 paste can be well predicted in terms of w/c, polymer content, and curing time using four various
45 simulation techniques. Among the used approaches and based on the training data set, the model
46 made based on the Non-linear regression, ANN, and M5P-tree models seem to be the most
47 reliable models. The sensitivity investigation concludes that the polymer content is the most
48 dominating parameter for the prediction of the compression strength of cement paste with this
49 data set.

50 **Words of key:** Cement paste; Polymer contents; Strength; Statistical analysis; Modelling.

51 **1. Introduction**

52 Cement plays an adhesive role in binding materials used in Construction Engineering. Cement is
53 widely used in construction and well-cemented oil fields. Cement alone (neat) can be used as
54 grouting, mortar and concrete processing, pipe joints, and foundation preparation [1]. Calcium
55 (sand or clay), aluminum, and iron are the main raw materials for cement production. The
56 chemical properties of the cement and its time change provide insight into the strength of the

57 cement system and the chemical properties of cement [2, 3, 4]. A variety of byproduct products
58 used in many comprehensive research trials to alter the properties of cement-based concrete such
59 as slag, calcinated clay, calcined clay, fuel ash, husk ash, soil granulated furnace slag, and
60 metakaolin [8, 11-15]. Polycarboxylates were utilized to modify concrete by accelerator or to
61 delay the setting time following the desired project to increase the viscosity and mechanical
62 behavior in liquid and solid phases by reducing water mixing [16-18]. The addition of polymeric
63 additives to the cement grid optimizes the viscosity, fluidity, and strength properties through the
64 development of an electrostatic distaste and stress-causing deflocculating [18-20]. The
65 application of small amounts of polymer admixture in cement increases the water content needed
66 to achieve the desired flowability [21, 22]. When the cement layer has been in contact with water
67 molecules, polycarboxylate, and other ions are found in the saturation zone [18]. The mixing
68 water and cement particles adsorption on the interface has been fixed by polycarboxylate ether
69 molecules that cause a negative charge around each cement particle [19-24].

70 There are several methods for modeling the properties of materials, including computational
71 modeling, statistical techniques, and recently developed tools such as regression analyses and
72 Artificial Neural Networks (ANN) [25, 26]. Multilinear regression analysis, M5P-tree, and ANN
73 are techniques widely used to solve problems in construction project applications [27-38]. The
74 most important characteristics of ANN is the ability to learn directly from examples and the great
75 response to imperfect tasks. An ANN, as opposed to traditional programming-based computing,
76 is a mathematical model or a computational model based on brain-like learning. The model
77 consists of interconnected artificial neuron groups that stimulate the brain structure to store and
78 use knowledge and process information using a connectionist approach [39-41]. Feedforward
79 networks, also known as multilayer perceptron, are the most common ANN models for many

80 applications. Most of the attempts have been related to a single scale model without covering a
81 wide experimental data or multiple parameters [42, 43, 44]. Thus, the effect of several
82 parameters such as the polymer content, w/c and curing time of 1 day up to 28 days was
83 quantified using different model techniques, namely linear and non-linear regressions, M5P-tree
84 and ANN-based approaches for predicting the compression strength of cement paste using 280
85 tested samples.

86 **1.1. Research significant**

87 The main objective of this study is to propose systematic multiscale models to predict the
88 compression strength of cement paste containing polymers. Thus, a wide experimental data (280
89 tested samples with different polymer contents, curing period and ratio between water to cement)
90 was considered with different analysis approaches (i) to guarantee the construction industry to
91 use the proposed models without any theoretical; (ii) to perform a statistical analysis and
92 understand the effect of the composition of the cement paste such as polymer content, and the
93 ratio between water to cement on the compression strength of the cement paste; (iii) to quantify
94 and propose a systematic multiscale model to predict the compression strength of cement paste
95 containing small amounts of polymers (up to 0.16%) with various water-to-cement ratio and
96 curing time up to 28 days; (iv) to find the most reliable model to predict the compression
97 strength of cement paste from four different model techniques (linear, nonlinear relations, M5P-
98 tree, and ANN models.) using statistical evaluation parameters.

99 **2. Methodology**

100 The tests were conducted following ASTM and British standards. For each case, an average of
101 three samples is considered.

102 **2.1 Ordinary Portland Cement**

103 In this research, the Ordinary Portland Cement (OPC) from the Gasin Cement Company was
104 used. The chemical and mineralogical components of the cement used are shown in Fig. 1.
105 Based on the SEM test the cement particle size was varied between 14.4 μm to 42 μm as shown
106 in Fig. 2(a).

107 **2.2 Polymers**

108 Two types of water-reducing polymer (Synthetic powder) were used. The commercial label of
109 the used polymers is DBC-21(Polymer 1) and VK-98 (Polymer 2). The properties of the two
110 types of polymer are listed in Table 1. From the SEM test, the polymer 1 had a rough or fibers
111 surface (Fig. 2(b)) while the polymer 2 had a smooth surface (Fig. 2(c)). The polymer particles
112 have an attractive property to each other and the particles of different materials.

113 **2.3. X-ray**

114 Analysis of the composition of chemical substances of cement at 25°C was conducted for X-ray
115 diffraction (XRD). The XRD pattern of particles was obtained by a Siemens D5000 X-ray
116 diffraction system. The samples were analyzed by using parallel beam optics with $\text{CuK}\alpha$
117 radiation at 40 kV and 30 mA. The samples were scanned for reflections (2θ) from 0° to 90° in
118 steps of 0.02° and 2 sec count time per step. XRD was undertaken to detect the major chemical
119 and mineralogical component of cement. The main chemical and mineralogical formulation in
120 the cement included C_3S , C_2S , C_3A , C_4AF , and Quartz, (SiO_2) (see Fig. 1).

121 **2.4. Scanning Electron Microscope (SEM)**

122 An SEM quantum 400 from FEI Company was used in this paper. It is a high-resolution field
123 emission gun scanning electron microscope appropriate for imaging and analysis of nano-scale
124 size. The samples were prepared and put the specimen on the surface of the stamp. The
125 conductive tape was used on the surface of the stamp. The sample holder was seated into the

126 appropriate hole on the sample holder mount. The polymers and cement are tested in powder
127 condition and the cement modified with polymers was tested after 7 days of curing.

128 **2.5. Fluidity**

129 The fluidity of cement slurry was measured using the ASTM C-230 mini-slump cone testing
130 method. The top, bottom, and height of the cone respectively are 70 mm, 100 mm, and 60 mm.
131 The cement slurry distribution was 191 mm for a water-cement ratio of 0.5. The addition of
132 polymers decreased the water content of cement slurries but increased their fluidity by 7-26%
133 depending on the polymer type, the polymer percentage, and the amount of water-cement.

134 **2.6. Standard consistency test**

135 The purpose of this study is to determine the minimum water mix to measure the initial chemical
136 reaction between water and cement. Cement is one of the products that require the right amount
137 of water to reach the requisite strength of cement. The norm accuracy was obtained based on the
138 standard EN 196-3. Polymers to reduce the amount of water required to achieve the same quality
139 (Fig. 3).

140 **2.7. Compression strength (ASTM C349)**

141 The cement paste after mixing is lined with cubic molds with a height of $(4 \times 4 \times 16) \text{ cm}^3$. The
142 cement paste put into the mold in one layer. After that, the mold is leveled and covered with a
143 plastic bag and stored at room temperature. After 24 hours the specimens were removed and
144 placed in the water at room temperature and 95 percent humidity, until the testing time. Samples
145 of compression strength were tested for 1, 3, 7, and 28 days. A $0.05 \text{ MPa}\cdot\text{sec}^{-1}$ flexural test
146 machine was used to separate the specimen into two parts and compressed each element at the
147 speed of $0.2 \text{ MPa}\cdot\text{sec}^{-1}$ using a compression machine (Fig.4) [45-52].

148 **2.8. Modeling**

149 The total tested of data (280 observations) was analyzed and divided into two groups. The larger
150 group included 187 data used to create models, while the other group included 93 data used to
151 validate models [53, 54]. The input data set consists of the water to cement ratio (w/c) the curing
152 age (t, days), and the polymer content (P, %), while the tested compression strength (MPa) for
153 the cement paste was used as a target. The following models (sections 2.8.1 -2.8.4) were used to
154 assess the impact of the mentioned parameters on the compression strength of the cement paste.

155 **2.8.1. Linear Approach (LR) Model**

156 LR model can be considered one of the most common regression equations (Eq.1) for the
157 prediction of cement [55].

$$158 \quad \sigma_c = a + b * (w/c) \quad (1)$$

159 where, σ_c , $\frac{w}{c}$, a, & b denote compression strength of cement paste (MPa), water to cement ratio,
160 and equation parameters, respectively. However, other cement paste components factors
161 affecting the compression strength, the type of cementitious materials, and curing time are not
162 included in the equation. To have more reliable results, Eq. 2 is proposed to include other factors.

$$163 \quad \sigma_c = a + b * (w/c) + c * (t) + d * (P) \quad (2)$$

164 Where: w/c is a water-to-cement ratio, t is curing age (days), and the Polymer content (P, %),
165 respectively, and the parameters of the model are a, b, c, and d. In compliance with Eq. 2, all the
166 variables seem to be adapted with linear (Eq. 1) extent. Nevertheless, this may not necessarily be
167 occurred for all cases because the variables involved in a cement paste mix may affect its
168 compression strength and interrelate with each other. Thus, it always needs to modify the model
169 to reliably predict the compression strength of cement paste with acceptable high accuracy [56-
170 58]. Accordingly, Eq. 2 was converted to a multivariable power equation.

171 **2.8.2. Nonlinear Regression Model (NLR)**

172

173 To develop a nonlinear regression model, the following formula (Eq. 3) can be considered as a
174 general form [41-49]. Eq. 3 is representing the interrelation between the variables given in Eq. 2
175 and Eq. 3 to estimate the compression strength of the conventional and cement paste component.

176
$$\sigma_c = a * \left(\frac{w}{c}\right)^b * (t)^c + d * \left(\frac{w}{c}\right)^e * (t)^f * (P)^g \quad (3)$$

177 **2.8.3 M5P-tree Model (M5P)**

178 M5P-tree is a genetic algorithm learner for regression problems, first introduced by a study [59].

179 This tree algorithm sets linear regression features on the terminal node and fits into a
180 multivariate linear regression model on each sublocation by classifying or dividing different
181 areas of data into multiple different-spaces. The M5P-tree approach is not discrete segments but
182 rather constant class problems and can handle rather high dimensional functions. Reveals the
183 data of every linear model component developed so that the nonlinear relationship of the data
184 sets is approximated. Error estimation is presented with information on the M5P-tree model tree
185 division criteria on each node. Errors measured by the default value variance of the class entering
186 the node. The attribute that maximizes the expected error reduction is used to evaluate any
187 function of that node. Information on the M5P-tree model tree dividing criteria is obtained based
188 on error calculations per node. The M5P error is determined by the standard deviation of the
189 class values at the node. The feature that maximizes the expected error reduction resulting from
190 evaluating each attribute at that node is chosen for node division. Due to the branching method,
191 child node data (subtree or smaller nodes) have less StDev. value. Parent nodes (greater nodes).
192 After reviewing all possible structures, select a system with the highest potential error reduction.
193 This division also creates a large tree-like structure that leads to overfitting. In the second step,

194 the enormous tree is pruned, and the trimmed subtrees are replaced by linear regression
195 functions.

196 **2.8.4. Artificial intelligence (ANN)**

197 ANN is a computing system that simulates the processes and analyses of the human brain. Also,
198 this model is a machine learning system used for various numerical predictions/problems in
199 Construction Engineering [60, 61]. ANN includes the input layer, the hidden layer (one or more
200 layers), and the output layer. The hidden layer is related by weight, transfer function, and bias to
201 the other layers. A multi-layer feed-forward network was programmed with a mixture of
202 proportions, w/c, curing time, and polymer content like inputs, and compression strength as
203 output. There is no standard method for designing or selecting a network architecture. Therefore,
204 the maximum number of hidden layers and neurons was calculated by the trial and error test
205 based on the lowest average square error criterion. The second step of the optimal network
206 design process was to choose the optimum number of epochs during the training that gave the
207 minimum MAE and RMSE and high R-value. The same preliminarily designed networks with
208 hyperbolic tangent transfer functions were used to see the effect of several epochs on reducing
209 the MAE and RMSE. The MAE variations with the number of epochs are presented for the
210 preliminarily designed networks. After designing the optimum architecture, the available data set
211 (total of 280 data) was divided into two parts; the first part was 2/3 of the overall data set (187)
212 for training the network, the second part was 1/3 of the total data set (93) for testing the network
213 [62]. Several transfer functions and ANN structures with a varied number of hidden layers and
214 neurons were tested to design the optimal network structure to predict the cement paste
215 compression strength. Among the networks, two hidden layers with eleven neurons with two
216 different neurons distributions and a hyperbolic tangent transfer function were chosen for the

217 cement paste modified with polymer 1 and polymer 2 due to having the minimum mean absolute
 218 error (MAE) as can be seen in Fig.5. In this part of the research, the ANN model was used to
 219 estimate the compression strength of polymer-containing cement paste as a cement replacement,
 220 w/c, curing time, and polymer contents.

221 **2.9. Model performance assessment criteria**

222 Correlation coefficients (R), mean absolute error (MAE), and root means square error (RMSE)
 223 values were used to estimate the ability of the above-mentioned modeling methods. Three
 224 common statistical measures: R, MAE, and RMSE were used as performance evaluation metrics
 225 to determine the efficacy of machine learning techniques. Numerous experiments were
 226 performed to determine the optimal value of key parameters. High R values (Eq. 4) and lower
 227 MAE values (Eq. 5), RMSE (Eq. 6) show better model precision.

$$228 \quad R = \frac{N \sum y_i x_i - (\sum y_i)(\sum x_i)}{\sqrt{N(\sum y_i^2) - (\sum y_i)^2} \sqrt{N(\sum x_i^2) - (\sum x_i)^2}} \quad (4)$$

$$229 \quad MAE = \frac{\sum_{i=1}^n |y_i - x_i|}{N} \quad (5)$$

$$230 \quad RMSE = \sqrt{\frac{\sum_{i=1}^n (y_i - x_i)^2}{N}} \quad (6)$$

231 y_i = tested data; x_i = predicted data; \bar{y} =mean value of y_i ; and N is the data set.

232 **3. Analysis and outputs**

233 **3.1. Scanning electron microscope**

234 The results for the OPC, polymers, and cement paste, modified with 0,06 percent polymers, were
 235 tested using a Scanning Electron Microscope (SEM) at seven days of curing (Fig. 5). Based on
 236 the SEM test analysis, the polymers samples were amorphous [63]. Fig. 2(a) showed that the
 237 cement particle size has varied particle sizes ranging between 14.4 μm to 42 μm . Fig.
 238 2(b) showed that most of the polymer 1 particles reposed of near-spherical with rough or fibers

239 surfaces. Most of polymer 2 particles also consisted of near-spherical but were very smooth as
240 compared to polymer 1 (Fig. 2(c)).

241 **3.2.Consistency**

242 Consistency is called the required amount of water combined to cause the chemical initial
243 reaction between water and cement. The use of polycarboxylate polymer on cement paste limited
244 the water that was needed to reach the required fluidity using mini-slump cone test outcomes.
245 The application of polymers (1&2) and cement decreased the needed water by 3 to 14 percent,
246 respectively, to the normal consistency. Polymers reduced water content by 24% to 66.3%
247 depending on the polymer type, polymer density (contains), fluidity, and w/c. The addition of
248 0.12% of polymer lowered w/c by 38% to 56% depending on the types of polymer, w/c, and
249 fluidity forms. The flow of cement paste was 290 mm and 430 mm w / c 0.6 and 1 respectively
250 while adding polymer simultaneously reducing the water content of cement paste and increasing
251 the fluidity by 1 to 8% depending on polymer type, polymer content and w/c.

252 **3.3.Water reducing, (WR)**

253 From the mini-slump, cone test results adding polycarboxylate polymer to the cement slurry
254 reduced the water required to reach the desired flowability. The addition of polymers reduced the
255 water content by 12.5% to 46.3% depending on the type of polymer, polymer percent, and
256 fluidity. The water to cement ratio of control sample 0.5. An additional of 0.04% of polymer
257 reduced the water-cement ratio by 25% to 32.5% depending on the types of polymer, water-
258 cement-ratio, and fluidity (Fig. 3 a). Based on the results of mini-slump cone tests, the addition
259 of polycarboxylate polymer to cement decreased the water needed for the fluidity necessary. The
260 addition of 0.12% polymer decreased the w/c by 38% to 56% based on the types of polymers,
261 w/c, and fluidity shown in Fig. 3(b).

262 **3.4. Compression strength**

263 The additional polymers were highly affected by increasing the compression strength (σ_c) of
264 cement paste up to 28 days of curing. With the increase in the percentage of polymer (P %) the
265 compression strength of cement paste is nonlinearly increased. At 1 day of curing an additional
266 of 0.06 % of polymer 1 and 2 improved the compression strength of cement paste by 224% and
267 140% respectively. The addition of 0.06 % of polymer improved the σ_c of cement paste by 84 %
268 and 224% based on the types of polymer, water-cement ratio, and curing period. The
269 improvement is due to the presence of amorphous gel that filling spaces between cement
270 particles with fiber nets (netting) around the cement particles which lead to decrease voids and
271 binding the cement particle together leading to an increase in the compression strength of cement
272 paste (Fig. 7). For the initial w/c of 0.6 and 1 respectively, the compression strength of the
273 cement paste on 1 day of cure was 5.92 MPa to 3.98 MPa. With 0.08% addition of P1 and P2,
274 the compression strength of cement pastes improved by 90% to 544%, based on the polymer
275 content, type of polymer, and w/c (Fig. 7 and Fig. 8). By adding 0.16% P1 and P2 the
276 compression strength of the cement paste was raised by 229% to 361% at 28 days of treatment
277 based on polymer content and w/c (Fig. 7, Fig. 8, and Fig. 9). The experimental results show that
278 the presence of polymers in cement paste increases the compression strength of the cement paste
279 with confidence. The strength increases were due to the dispersal of cement particles and the
280 tensile bonding of particles, resulting in a reduction in the porosity and void ratio of cement paste
281 [52, 63].

282

283 **3.5.The relation between calculated and actual cement paste compression strength**

284 **(a) The linear model (LR)**

285 The model parameter observed that the w/c significantly decrease cement paste's compression
286 strength. Table 2 summarizes model parameters, R, MAE and RMSE, and data number. The
287 relationships between actual and calculated compression strength of the cement paste are shown
288 in Fig. 10. The research dataset contains a $\pm 35\%$ and $\pm 30\%$ error lines for the cement paste
289 treated with polymers (1&2) respectively, indicating that most checked results are in $\pm 35\%$ and
290 30% error lines, respectively (Fig. 10). Nevertheless, the model slightly underestimated the
291 strength cement paste ranged between 20 MPa to 40 MPa mixes.

$$292 \sigma_c = -50.25 - 63.85 * \frac{w}{c} + 1.06 * t + 100.86 * P_1 \quad (7)$$

293 No. of data = 187, R = 0.794, RMSE = 14.159 MPa

$$294 \sigma_c = 50.47 - 57.63 * \frac{w}{c} + 0.86 * t + 95 * P_2 \quad (8)$$

295 No. of data = 187, R = 0.802, RMSE=12.839 MPa

296 And from model parameters in the Eq. 7 and Eq.8, It can be inferred that the polymer content has
297 the highest impact on the compression strength of other w/c and curing time. According to
298 equation variables in the Eq.7 and Eq. 8 (d=100.86 and d= 95), Polymer 1 was much more
299 successful than polymer 2 for increasing the strength of the cement paste compression and the
300 simulation results with the same experimental results.Eq.7 and Eq.8 were also checked with the
301 research dataset as seen in Fig. 11.

302 **(b) Nonlinear Regression (NLR) Model**

303 The model parameter shows that cement content significantly influences cement paste's
304 compression strength. Clear relationships between calculated and actual compression strength

305 can be seen in Fig. 12. The study training dataset contains an error line of $\pm 25\%$ for the
 306 compression strength of the cement paste modified with P1 and P2, indicating that almost all
 307 checked results are in $\pm 25\%$ error lines. This model seems to be more reliable than LR to predict
 308 the compression strength of cement paste.

$$309 \quad \sigma_c = 10.55 * \frac{w^{-0.56}}{c} * t^{0.26} + 3.37 \left(\frac{t^{0.18} * P1^{0.21}}{\frac{w^{1.96}}{c}} \right) \quad (9)$$

310 No. of data = 187, R = 0.961, RMSE= 6.396 MPa

$$311 \quad \sigma_c = 12 * \left(\frac{t^{0.21}}{w^{0.52}} \right) + 3.21 * \left(\frac{t^{0.18} P2^{0.31}}{w/c^{2.14}} \right) \quad (10)$$

312 No. of data = 187, R = 0.924, RMSE= 8.235 MPa

313 Focusing on model parameters Eq.9 and Eq. 10, the maximum influence of polymer contents on
 314 increasing compression strength relative to other cement paste compositions can be obtained.
 315 Also based on the model parameters in the Eq.9 and Eq. 10 (d=3.37 and d= 3.21), the polymer 1
 316 was also more productive than the polymer 2 for enhance compression strength of the cement
 317 paste the similar observation was made in the experimental work. Eq. 9 and Eq.10 have also
 318 been validated using the testing dataset (Fig. 13).

319 (c) MSP-tree model

320 Fig. 14 shows the division of input space x_1, x_2 (independent variables) by the MSP-tree model
 321 algorithm into nine linear tree regression functions (marked LM1 through LM5). The model's
 322 general shape is $y = a_0 + a_1x_1 + a_2x_2$, where $a_0, a_1,$ and a_2 are linear regression constants.
 323 Fig.14 indicates the tree-shaped branch relationship and the model (Eq. 11) parameters are
 324 summarized in Table 3. The research dataset contains an error line of $\pm 30\%$ for the compression
 325 strength of the cement paste modified with P1 and P2, indicating that almost all measured results
 326 are in $\pm 30\%$ error lines (Fig. 15). Furthermore, the output of this model is more reliable than

327 those of the previous models. In other words, the calculated and actual compression strength of
328 the cement paste is adapted with the line of equality.

$$329 \quad \sigma_c = a * \left(\frac{w}{b}\right) + b * (t) + c * (P1) + d \quad (11)$$

330 No. of Data=187, R=0.950, RMSE= 7.354 MPa

$$331 \quad \sigma_c = a * \left(\frac{w}{b}\right) + b * (t) + c * (P2) + d \quad (12)$$

332 No. of Data=187, R=0.923, RMSE= 8.274 MPa

333 The model parameters (*a*, *b*, *c* and *d*), are listed in Table 3 and based on the linear tree
334 registration function (LM num:) the model variables will be selected. The models (Eq. 11 and
335 Eq. 12) have also been evaluated using the testing dataset as can be seen in Fig. 16.

336 **(d) ANN Model**

337 The network was equipped with the training data set, accompanied by the test data to predict the
338 compression strength values for the correct input parameters (Fig. 4). A sensitivity test for the
339 model predictions was also carried out for the cement paste modified with P1 and P2 (Fig. 17).
340 The ANN model based on the predictions over-predicted 93 of the data analyzed. A trial and
341 error cycle is the development of the ANN model (such as the number of hidden layer neurons,
342 number of hidden layers, momentum, learning rate, and iteration). The ANN model contains two
343 hidden layers for both polymers modified cement paste. Hidden layers contain 11 neurons and
344 three inputs with momentum = 0.2, learning rate = 0.1 and Iteration = 2000. The main concept to
345 generate data based on the ANN model is shown in Fig. 17. As summarized in Table 2, the ANN
346 model was obtained R = 0.986, MAE = 3.909 MPa, and RMSE = 4.743 MPa for the cement
347 paste modified with polymer 1 and R = 0.961, MAE = 4.309 MPa, and RMSE = 5.996 MPa for
348 the cement paste modified with polymer 2. The research dataset contains an error line of $\pm 20\%$
349 for both cement paste modifications, indicating that all measured results are in $\pm 20\%$ error lines.

350 The compression strength values calculated and the ANN expected are compared and validated
351 with the testing dataset in Fig. 17 and Fig.18. Overall, based on the results shown in Table 2 and
352 Fig. 17 and Fig.18, the accuracy of the ANN model is suitable for the prediction of compression
353 strength. Inter-comparison regression and soft computing-based models: Overall comparison
354 among Regression and soft computing-based models (Table 2) suggests that the ANN-based
355 model performs better than other applied models. NLR model is working better than the LR
356 model for this data set. Fig. 19 indicate the agreement plot and performance diagram both figures
357 suggest that the NLR and ANN-based model is outperforming than other applied models with
358 minimum deviation from agreement line or actual values. Three statistic parameters including
359 standard deviation, correlation, and root mean square error, evaluated the degree of compliance
360 of cement paste's compression strength among actual and predicted values.

361 **4. Sensitivity investigation**

362 A comparison between the sensitivity of the models was performed to evaluate the most
363 important input variable when calculating the cement paste's compression strength. Several
364 training data sets were created by extracting the single input variable at a time, and the test data
365 set reported the effects of R, MAE, and RMSE. Data set to split into two sections for training and
366 testing. The best performing model is selected for the sensitivity analysis. In this study, the
367 ANN-based model is used for sensitivity analysis. Results obtained from Table 4 indicate that
368 the polymer content is the most influencing parameter for the prediction of compression strength
369 using the M5Ptree-based model.

370 **5. Conclusions**

371 Based on the tested data and the simulation of the compression strength of cement paste at 280
372 different ratios between the water and the cement, polymer content, and curing ages, the
373 following conclusions are drawn.

- 374 1. The compression strength of cement increased by 84% to 360 % depending on the curing
375 time, water-cement ratio, curing time, and polymer contents. Based on NLR parameters,
376 polymer 1 (rough surfaces) had the highest impact on increasing the compression strength of
377 cement paste as compared to polymer 2 (smooth surfaces). This improvement of compression
378 strength was due to the dispersion of cement particles and increasing the friction between the
379 particles that lead to reduce the void ratio and increasing the density of cement paste.
- 380 2. From the SEM test analysis, the addition of the polymer produced a fiber net (netting) around
381 cement particle which leads to decrease void, binds the cement particles together, and
382 increased the compression strength of cement paste.
- 383 3. The designed ANN was used to predict the cement paste strength after it was trained by 2/3
384 of the 280 tested data. The ANN model predicted the compression strength of the testing data
385 with a reliable coefficient of correlation (R 0.968, 0.961). By using the same variables, a non-
386 linear relation (NLR) was derived and the parameters were found via multiple regression.
387 Similarly, the ANN model, NLR, and M5P-tree models have predicted the compression
388 strength of the testing data with a reliable coefficient of correlation.
- 389 4. Apart from the standard curing age, the results of this study have shown that the ANN model
390 is capable of predicting the 28th-days compression strength of cement paste. Based on the
391 training and testing data sets, the ANN and NLR models predicted the compression strength
392 very close to experimental data and the predictions were better than other models.

393 5. Sensitivity analysis showed that polymer content is the most important parameter for
394 predicting the compression strength of cement paste using the M5P-based model.

395 **Data Availability Statement**

396 No data, models, or codes were generated or used during the study.

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402 **Conflicts of Interest Statement**

403 None

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596

Figures

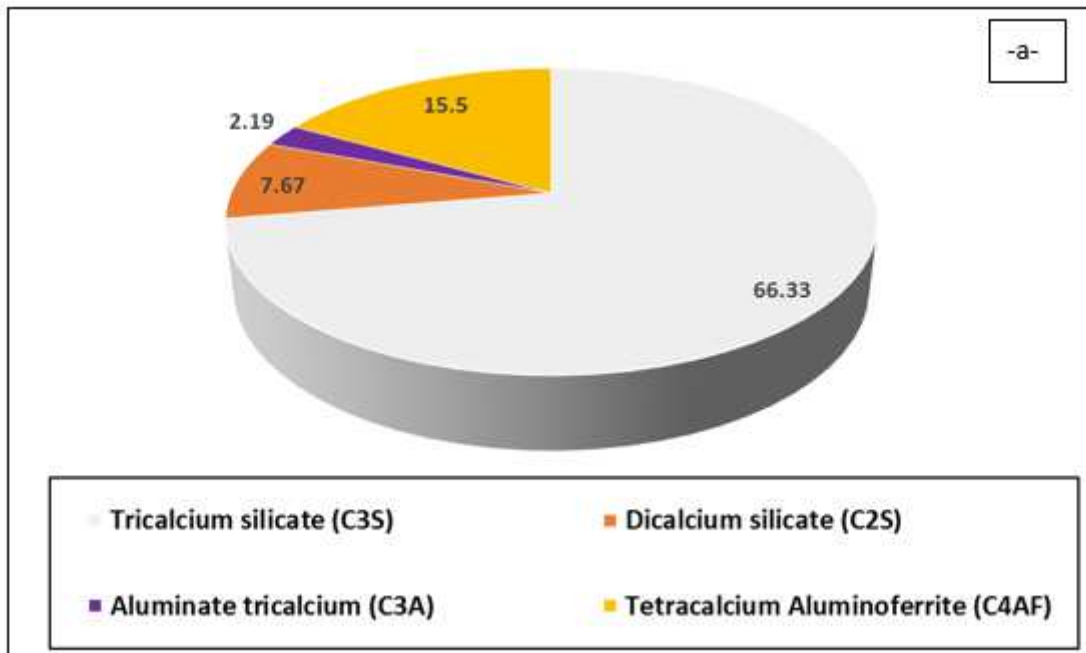
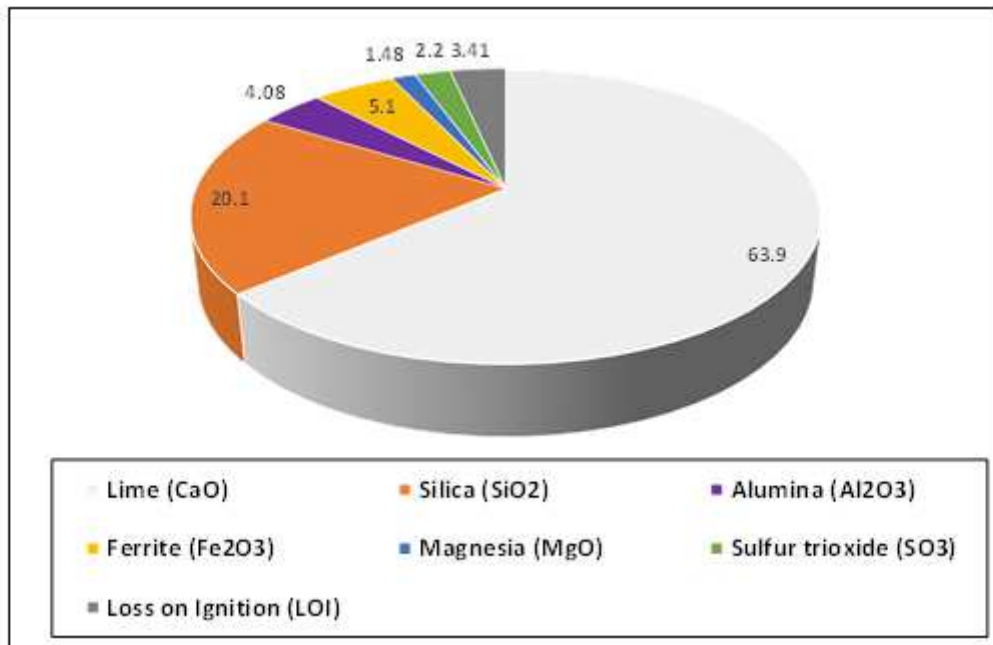


Figure 1

Percentages of (a) Mineralogical composition and (b) Chemical composition of the Ordinary Portland Cement (OPC)

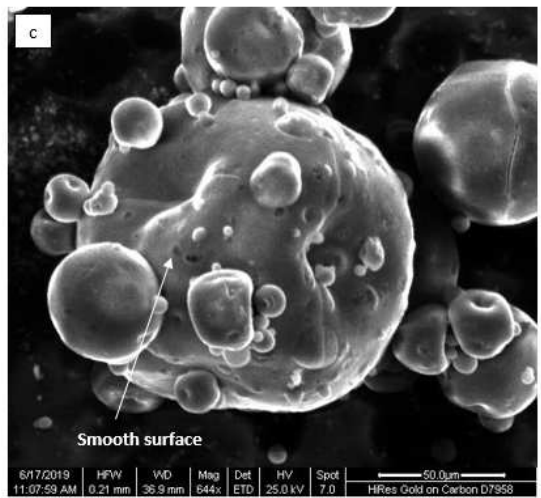
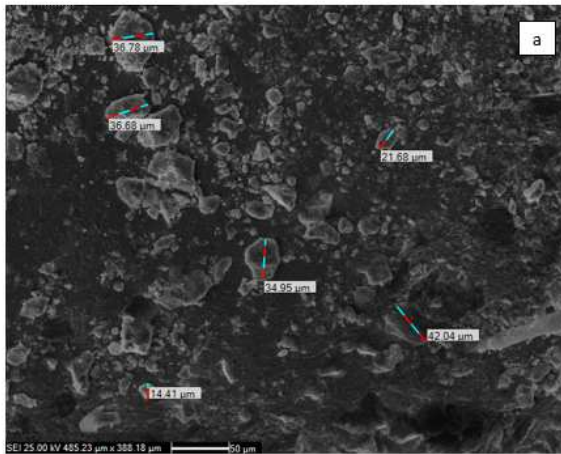
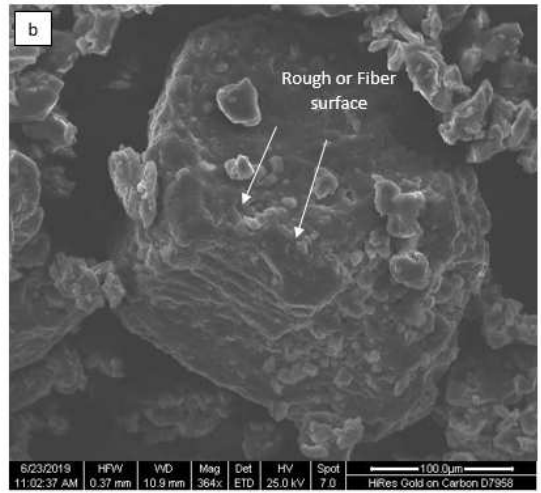
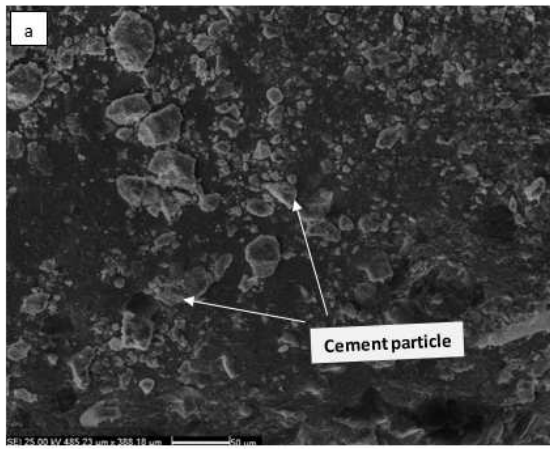


Figure 2

SEM test for (a) Ordinary Portland Cement (OPC) (b) Polymer 1 and (c) Polymer 2

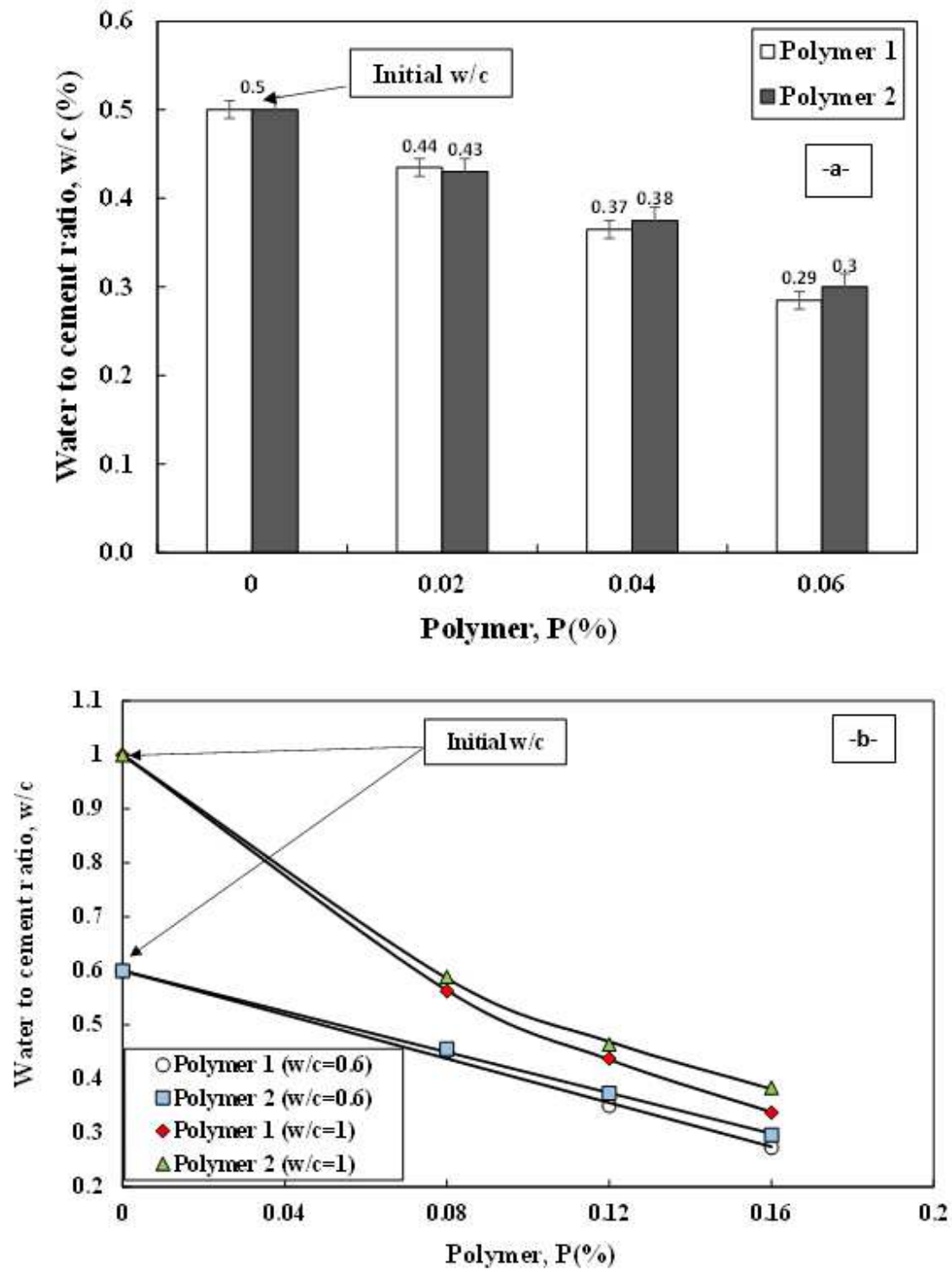


Figure 3

The variation between polymer content and water to cement ratio (w/c) of cement (a) initial w/c=0.5 and (b) initial w/c =0.6 and 1

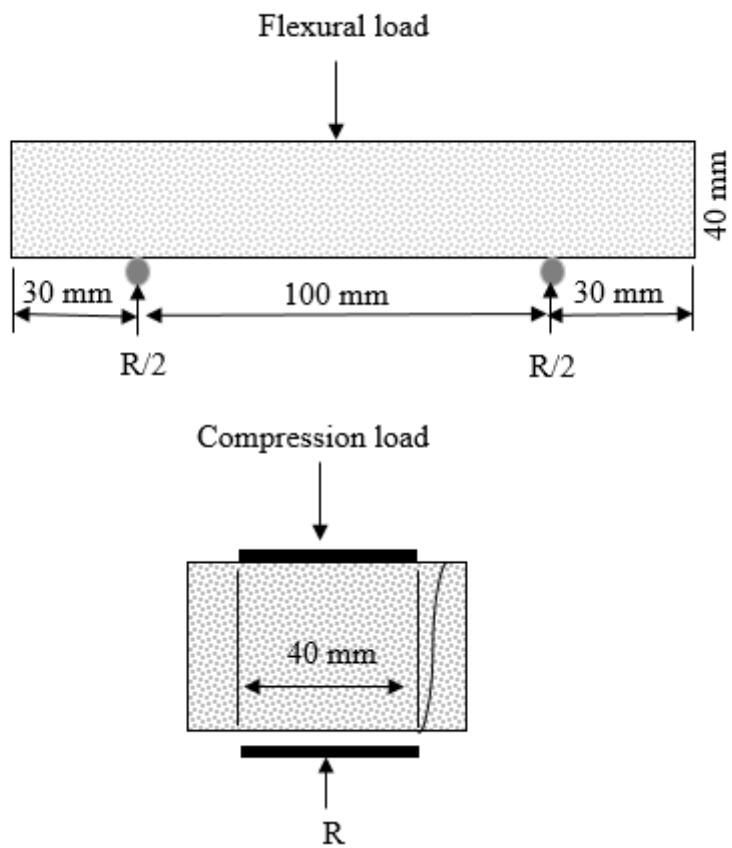


Figure 4

The layout of the cement specimen for a compression test

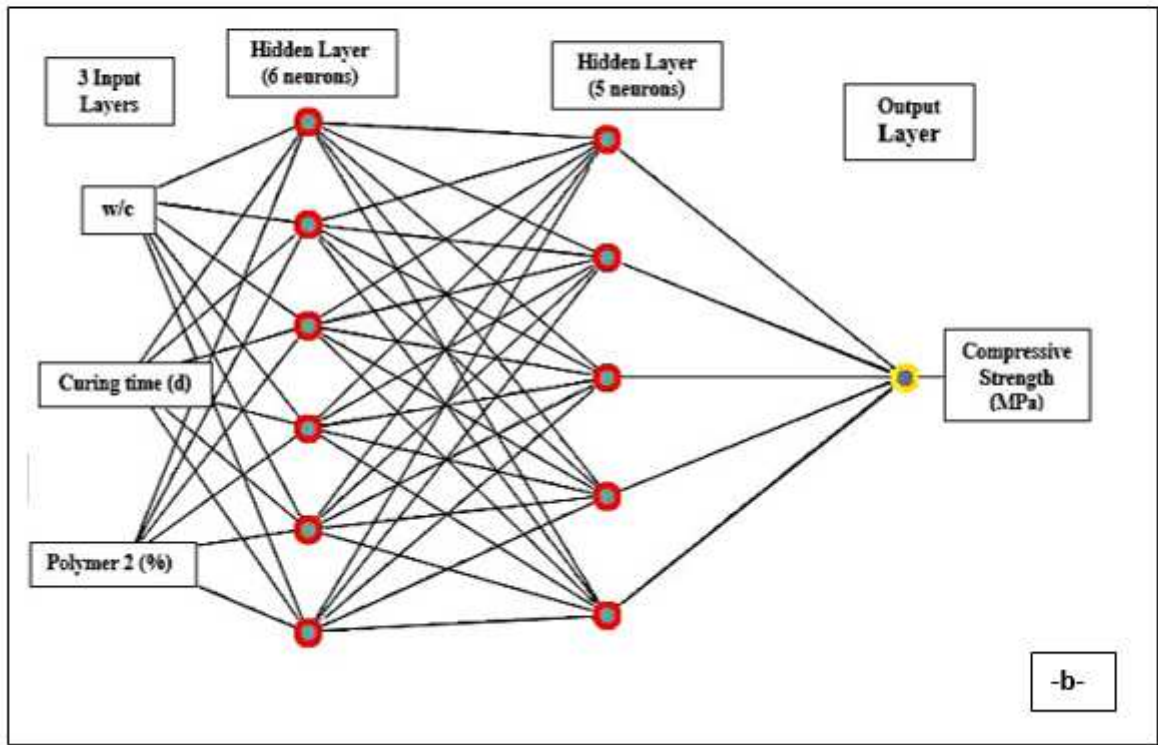
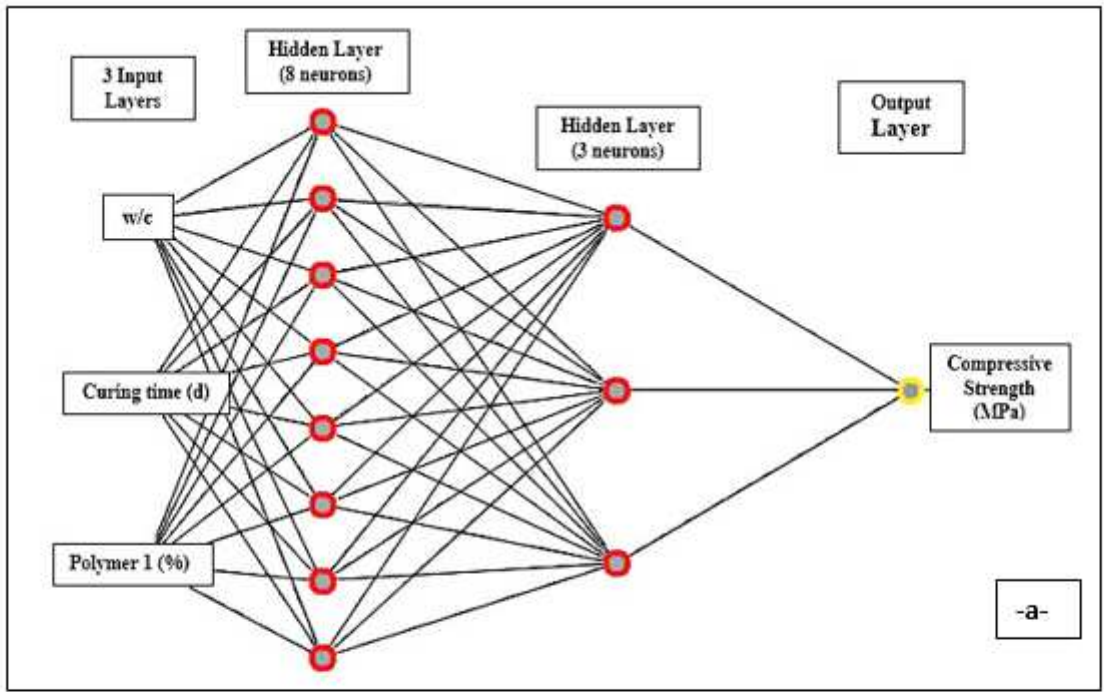


Figure 5

Optimal Network Structures of Neural Network Model (a) cement paste modified with Polymer 1 and (b) cement paste modified with Polymer 2

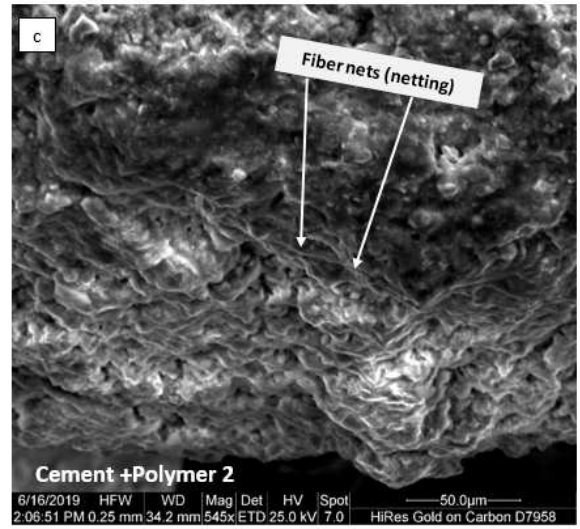
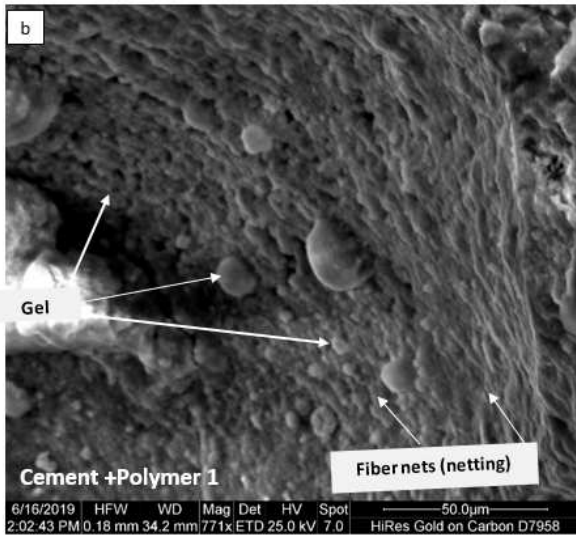
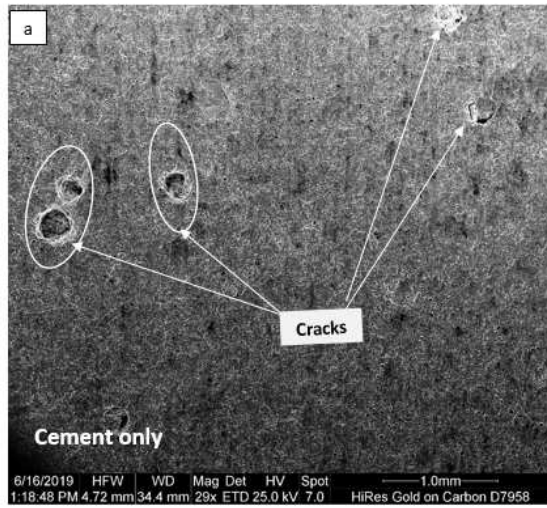


Figure 6

SEM test for (a) OPC (cement only) (b) Cement modified with 0.06% of polymer 1, and (c) Cement modified with 0.06% of polymer 2 after 7 days of curing

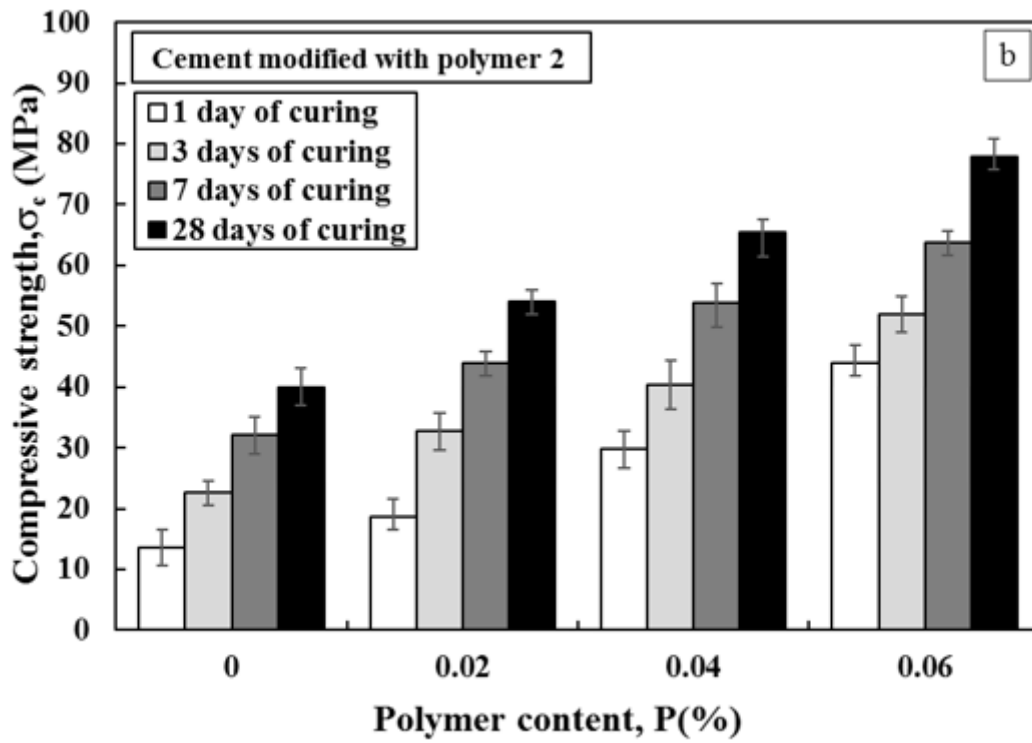
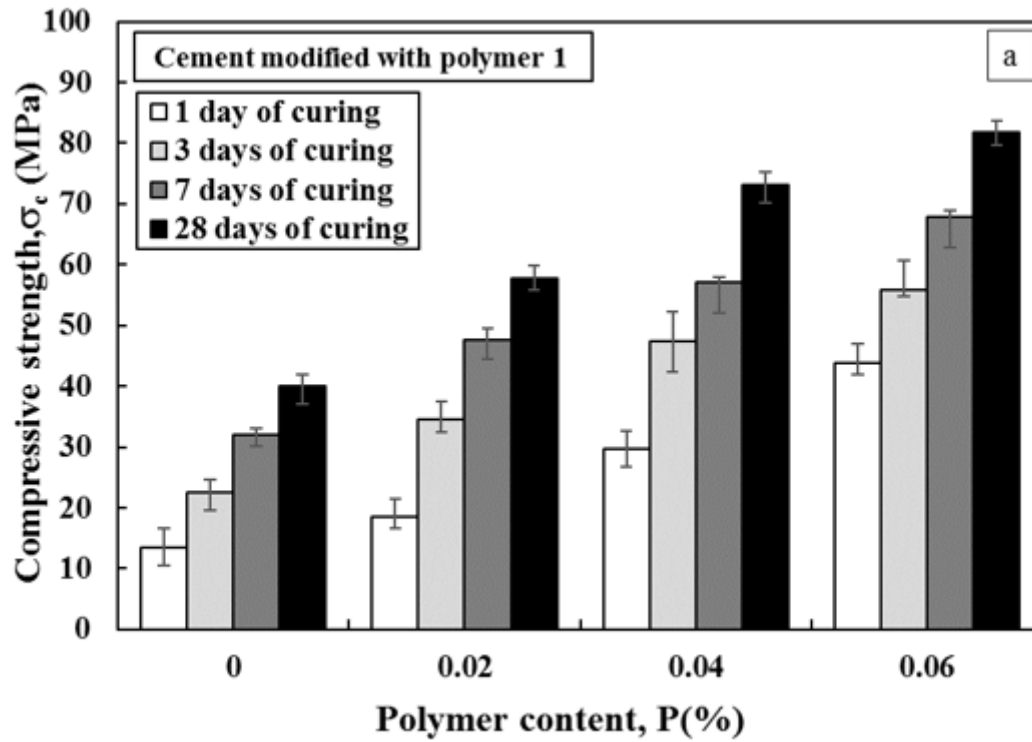


Figure 7

Variation of the compressive strength of cement paste and polymer contents at initial w/c of 0.5 (a) Polymer 1 and (b) Polymer 2 at different curing times

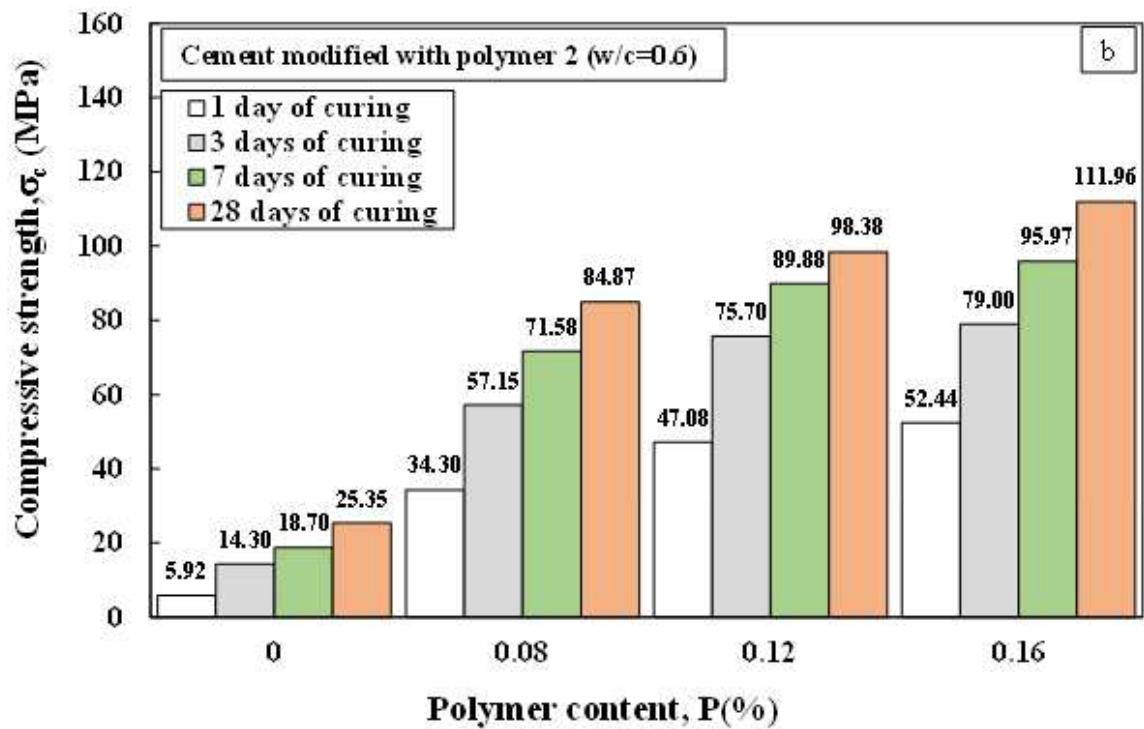
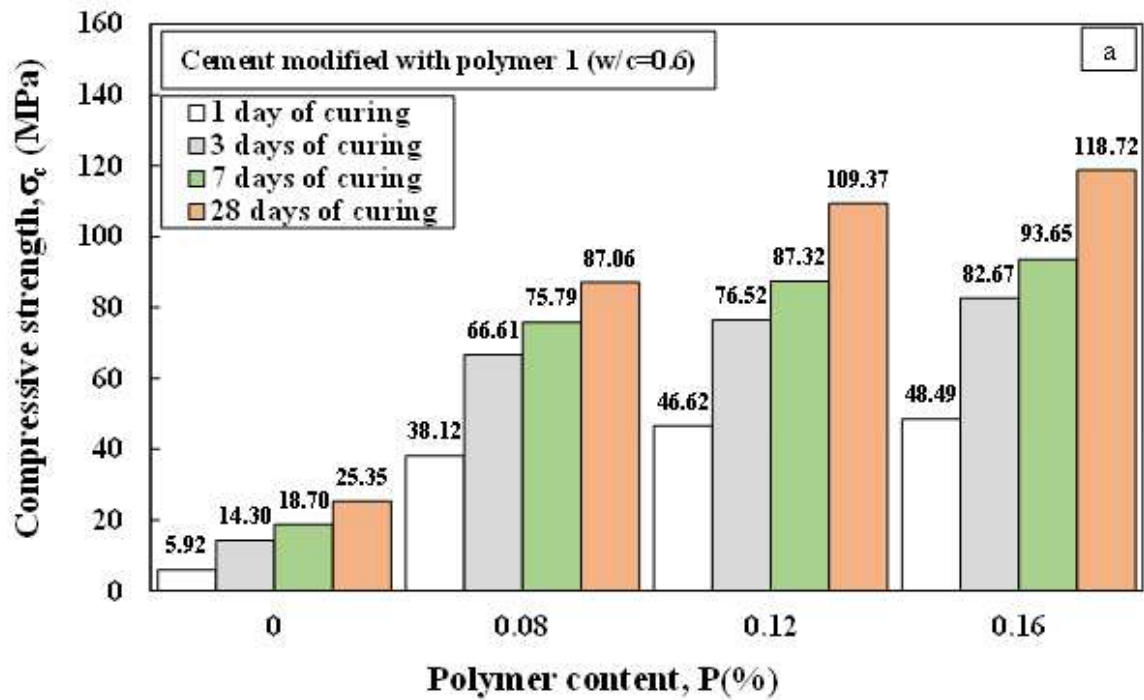


Figure 8

Variation of the compressive strength of cement paste and polymer contents at initial w/c of 0.6 (a) Polymer 1 and (b) Polymer 2 at different curing times

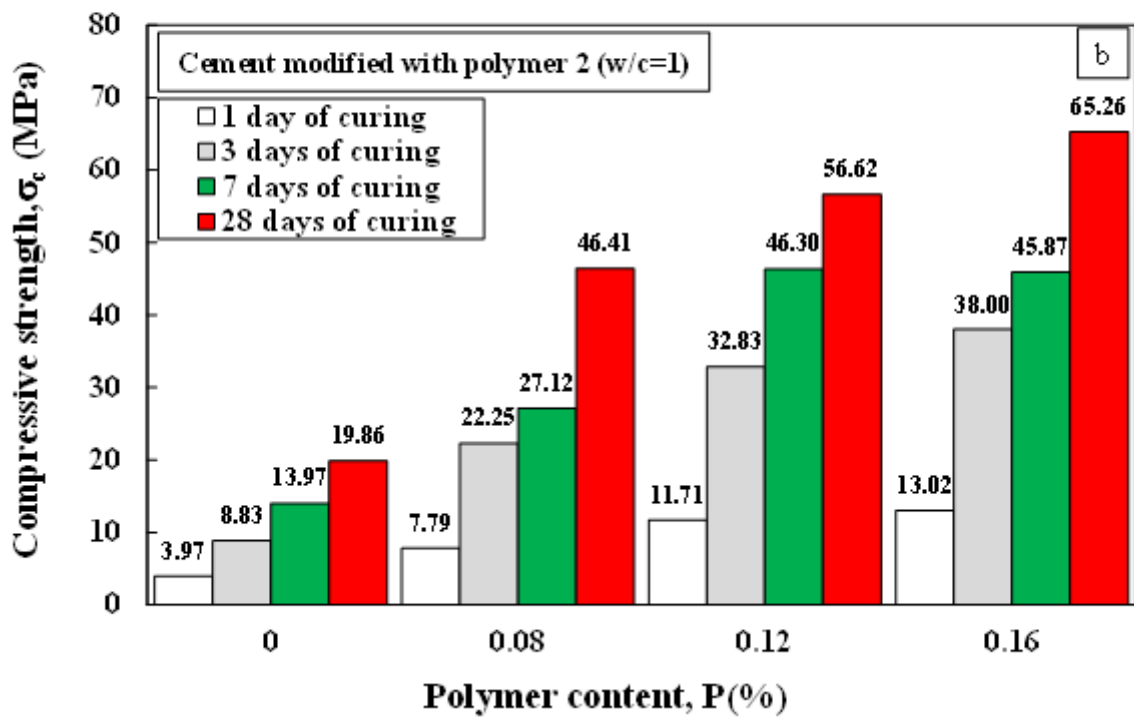
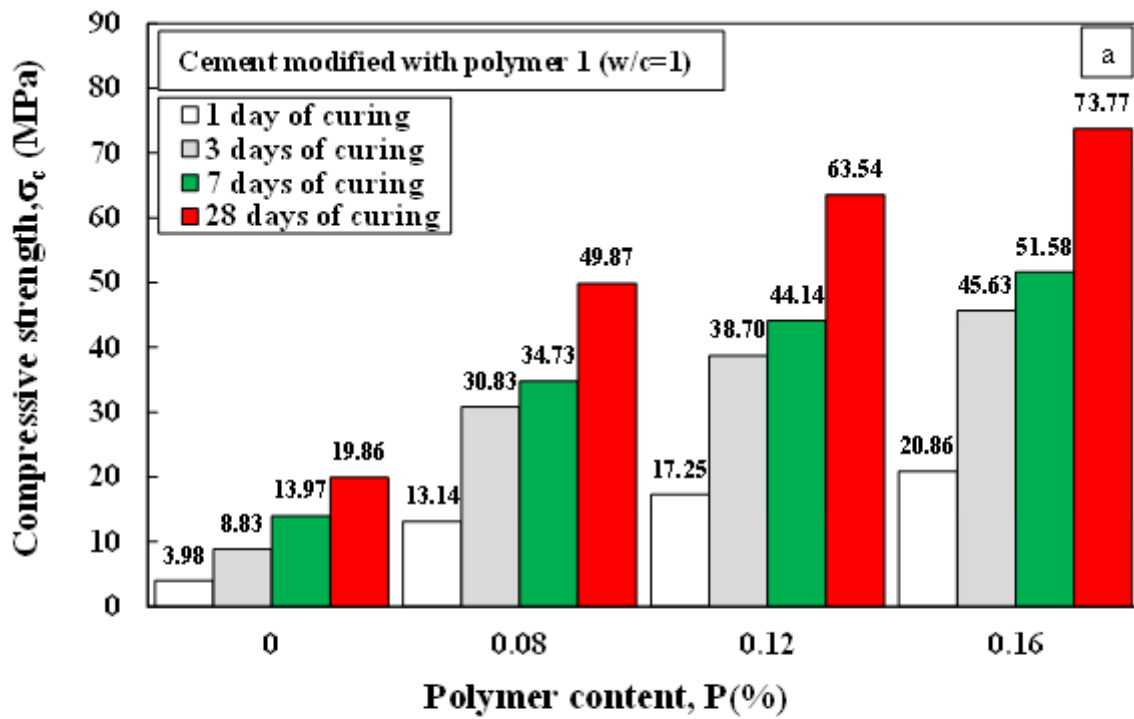


Figure 9

Variation of the compressive strength of cement paste and polymer contents at initial w/c of 1 (a) Polymer 1 and (b) Polymer 2 at different curing times

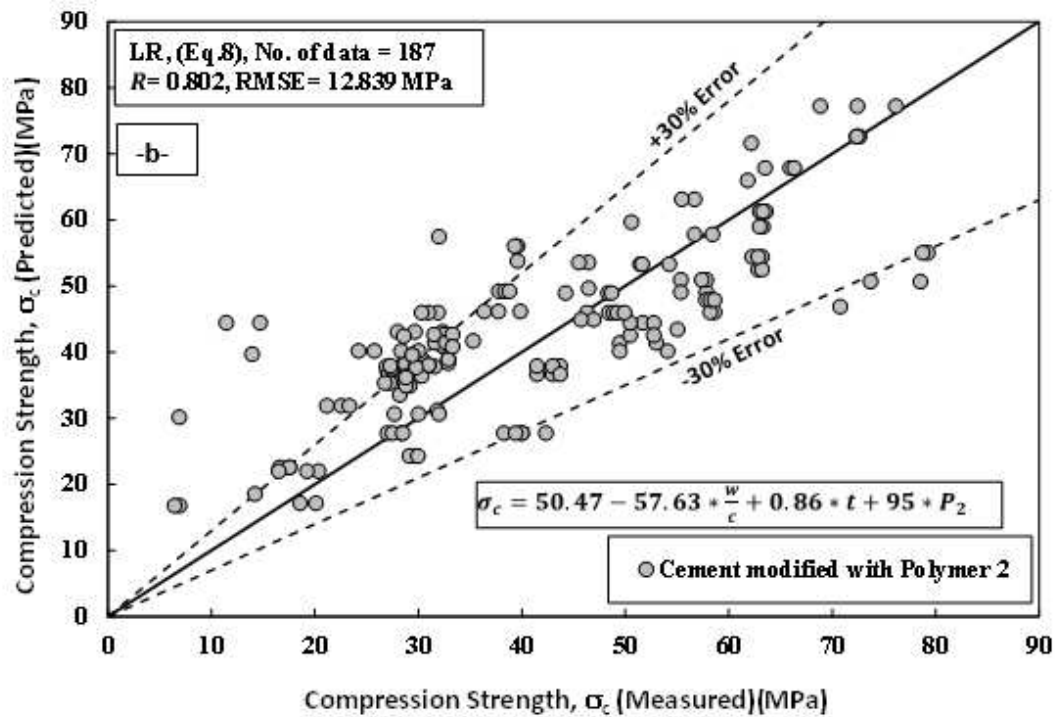
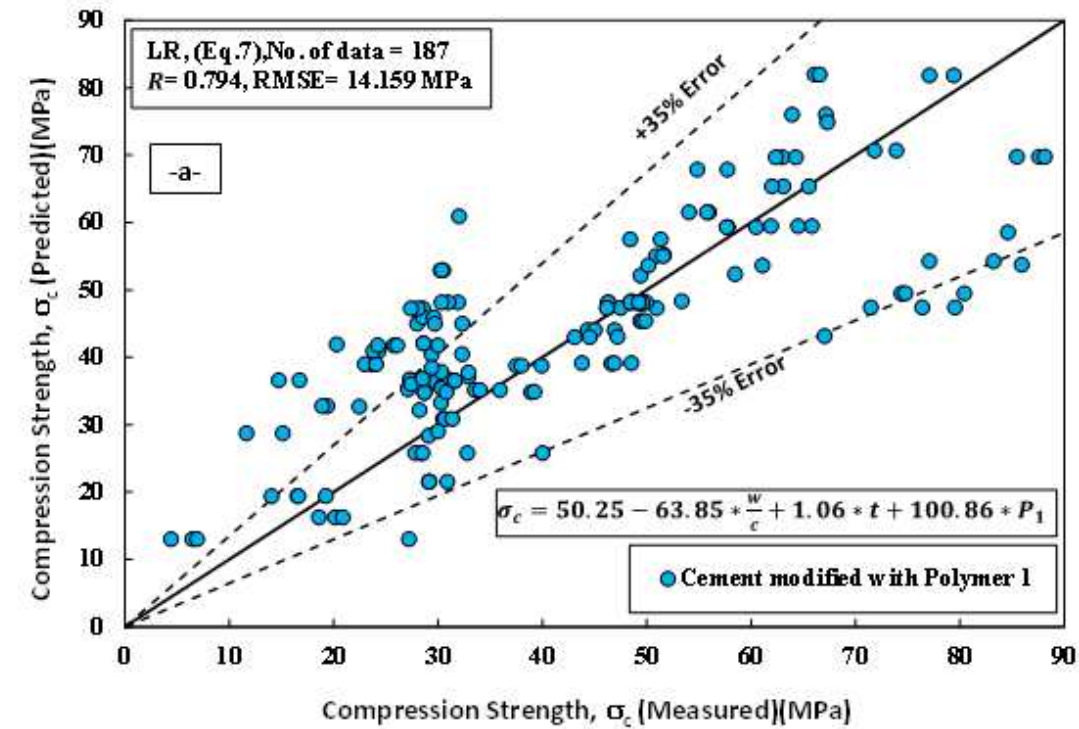


Figure 10

Comparison between measured and predicted the compressive strength of cement paste modified with polymers using Linear Regression Model (LR) for the training data (a) polymer 1, and (b) polymer 2

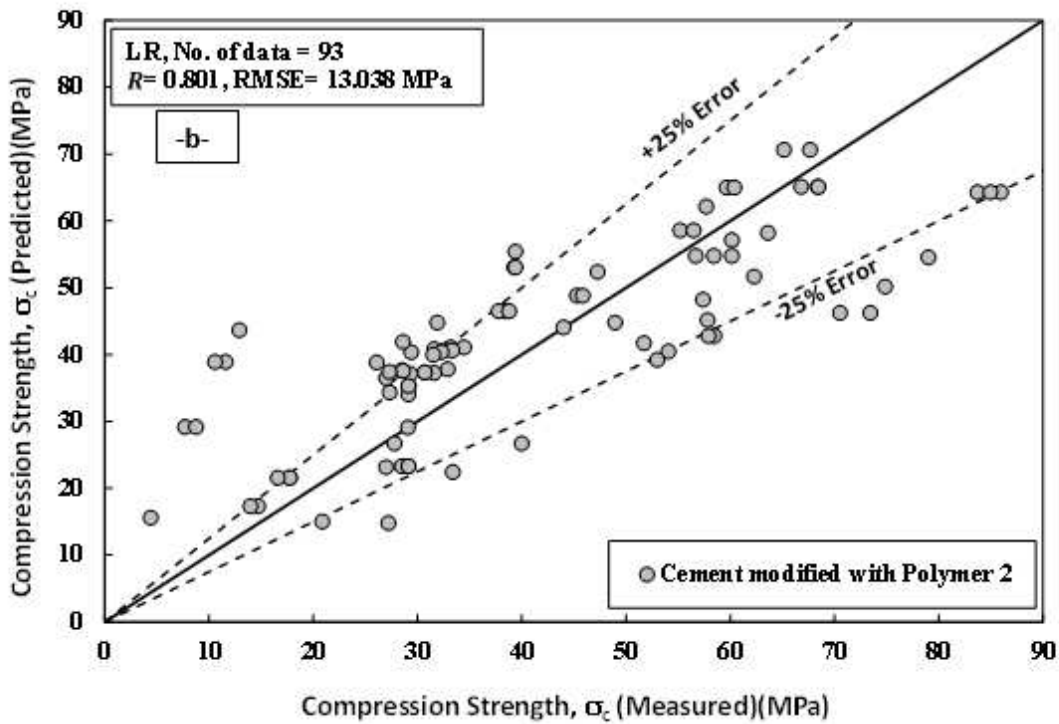
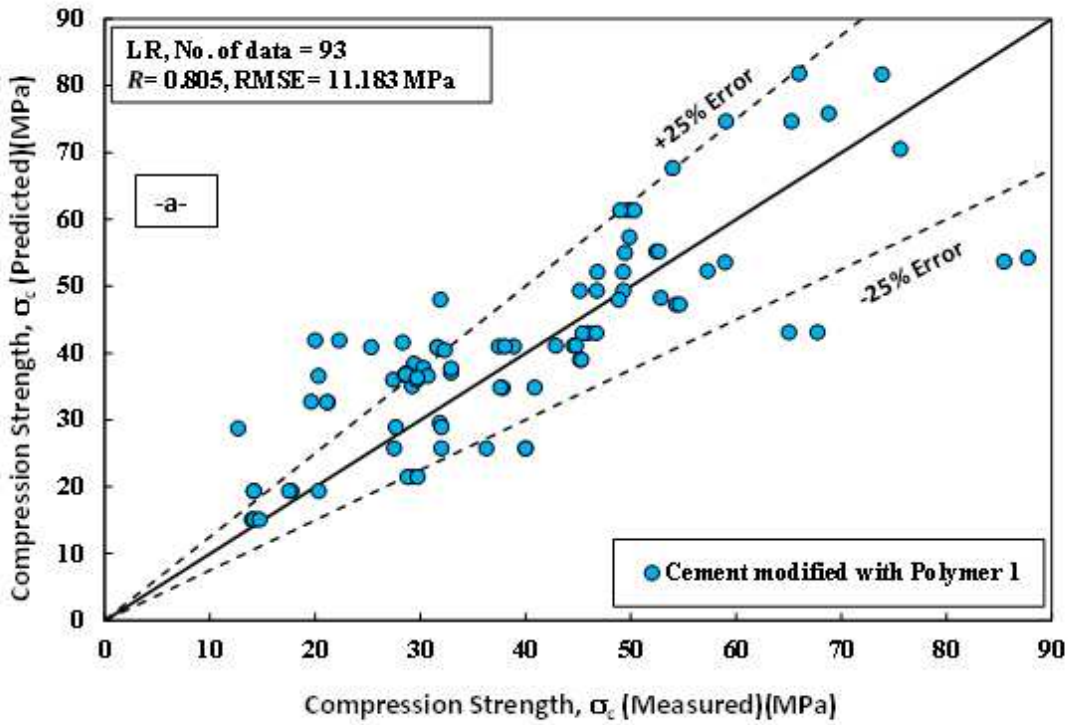


Figure 11

Comparison between measured and predicted the compressive strength of cement paste modified with polymers using Linear Regression Model (LR) for the testing data (a) polymer 1, and (b) polymer 2

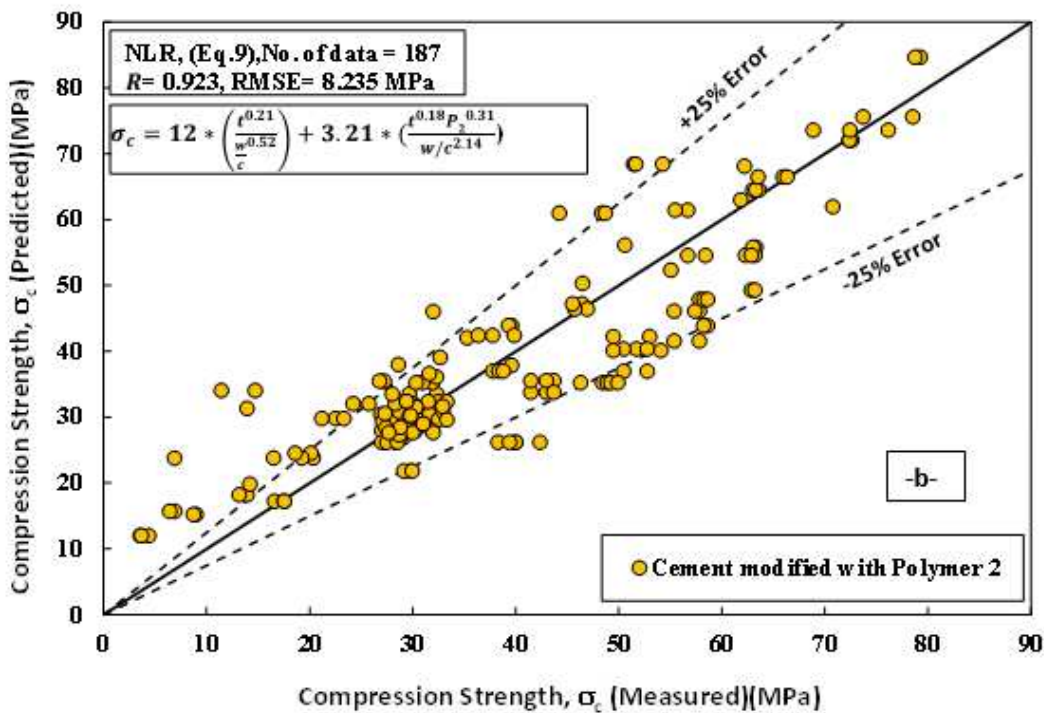
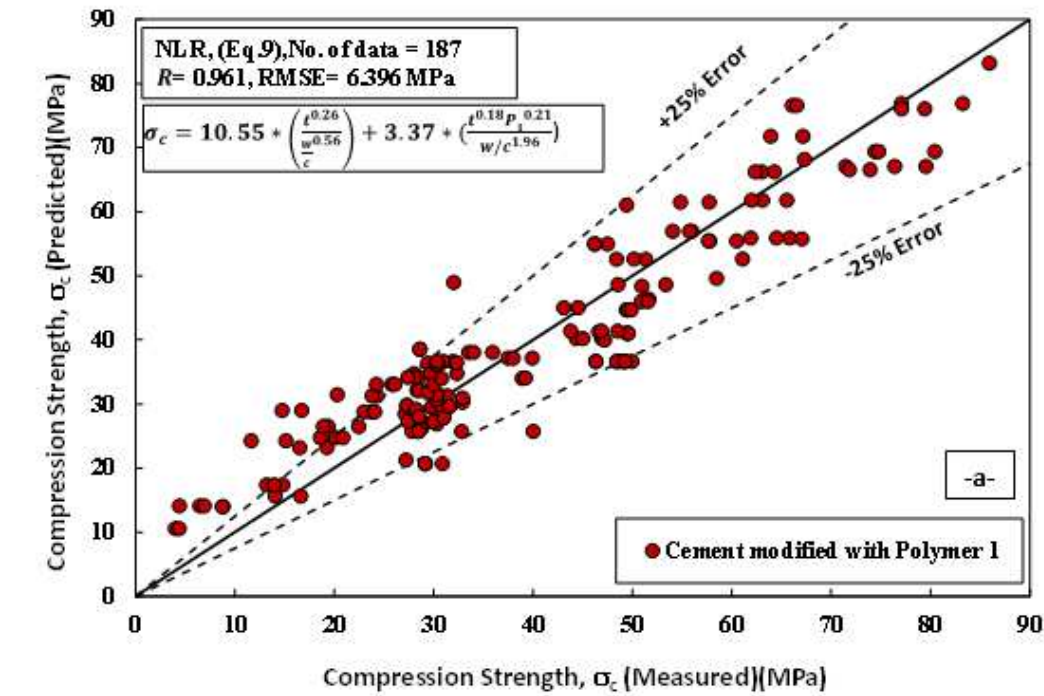


Figure 12

Comparison between measured and predicted the compressive strength of cement paste modified with polymers using Non-Linear Regression Model (NLR) for the training data (a) polymer 1, and (b) polymer 2

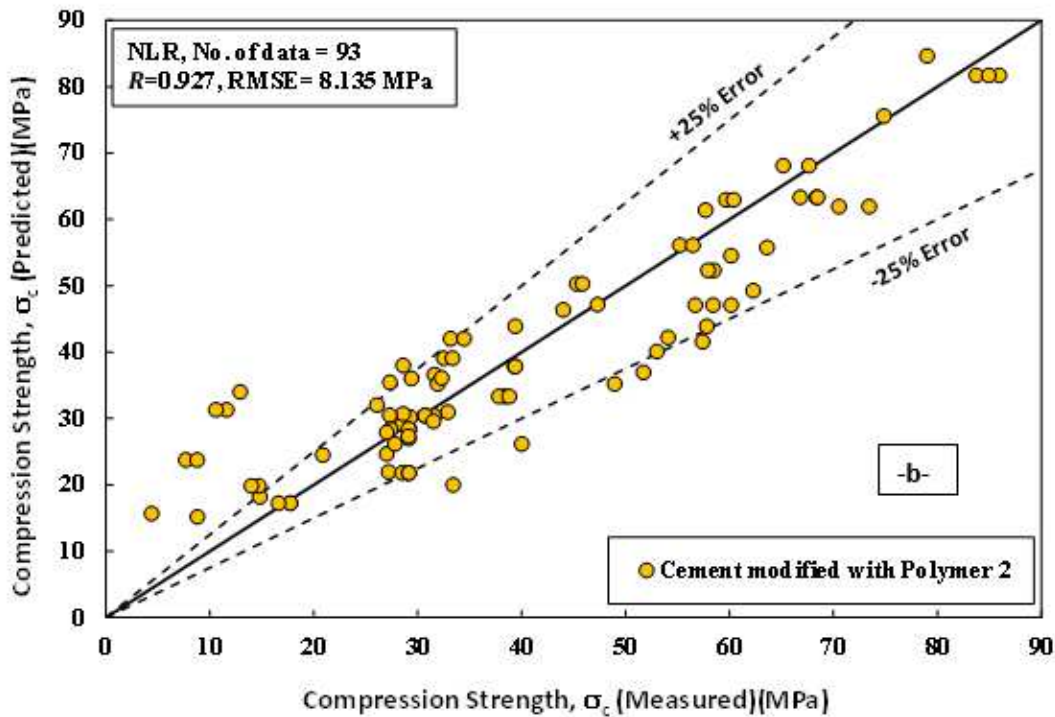
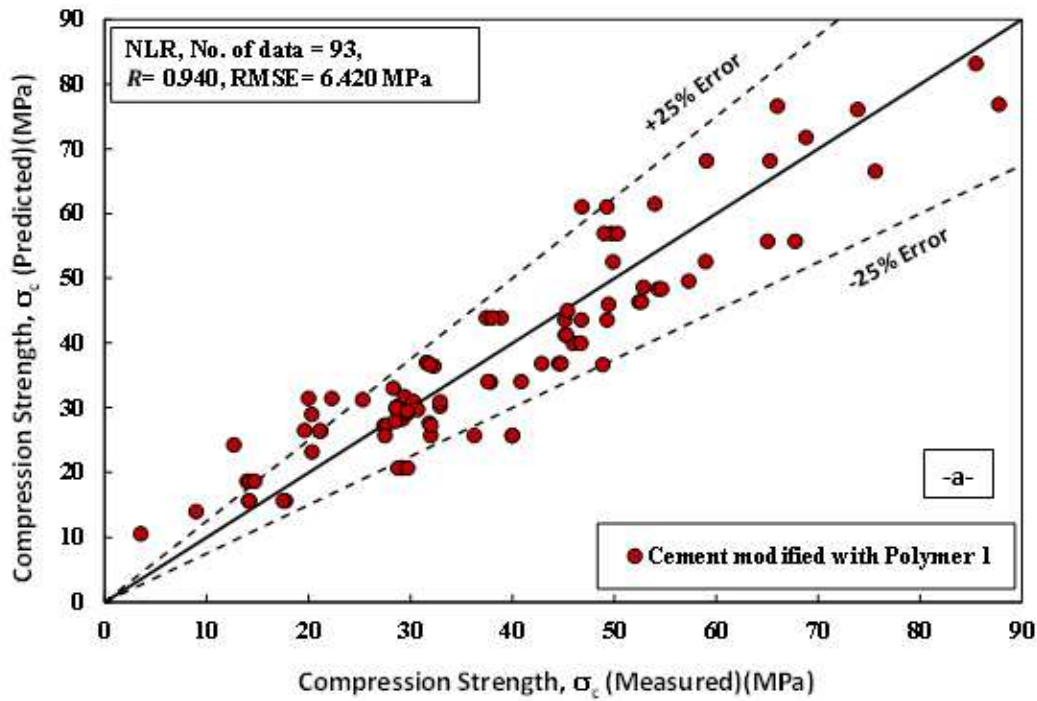


Figure 13

Comparison between measured and predicted the compressive strength of cement paste modified with polymers using Non-Linear Regression Model (NLR) for the resting data (a) polymer 1, and (b) polymer 2

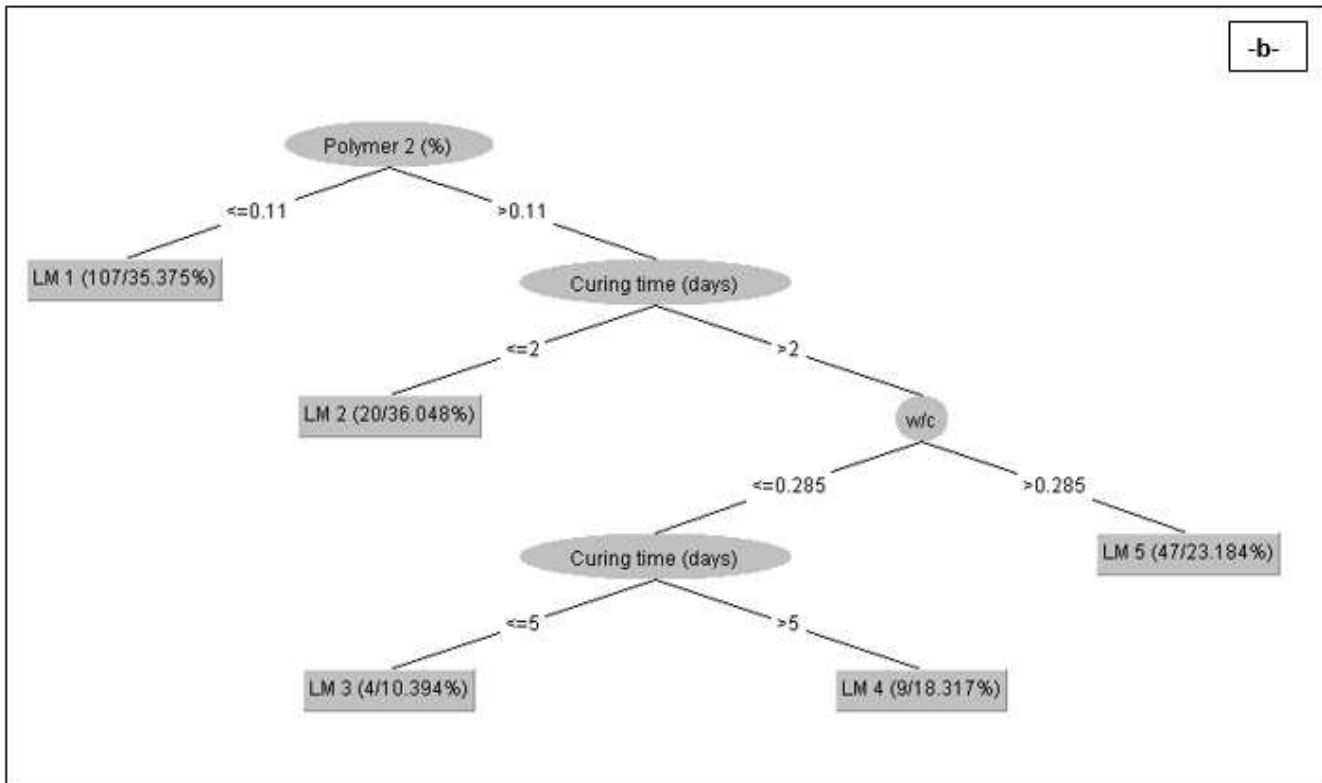
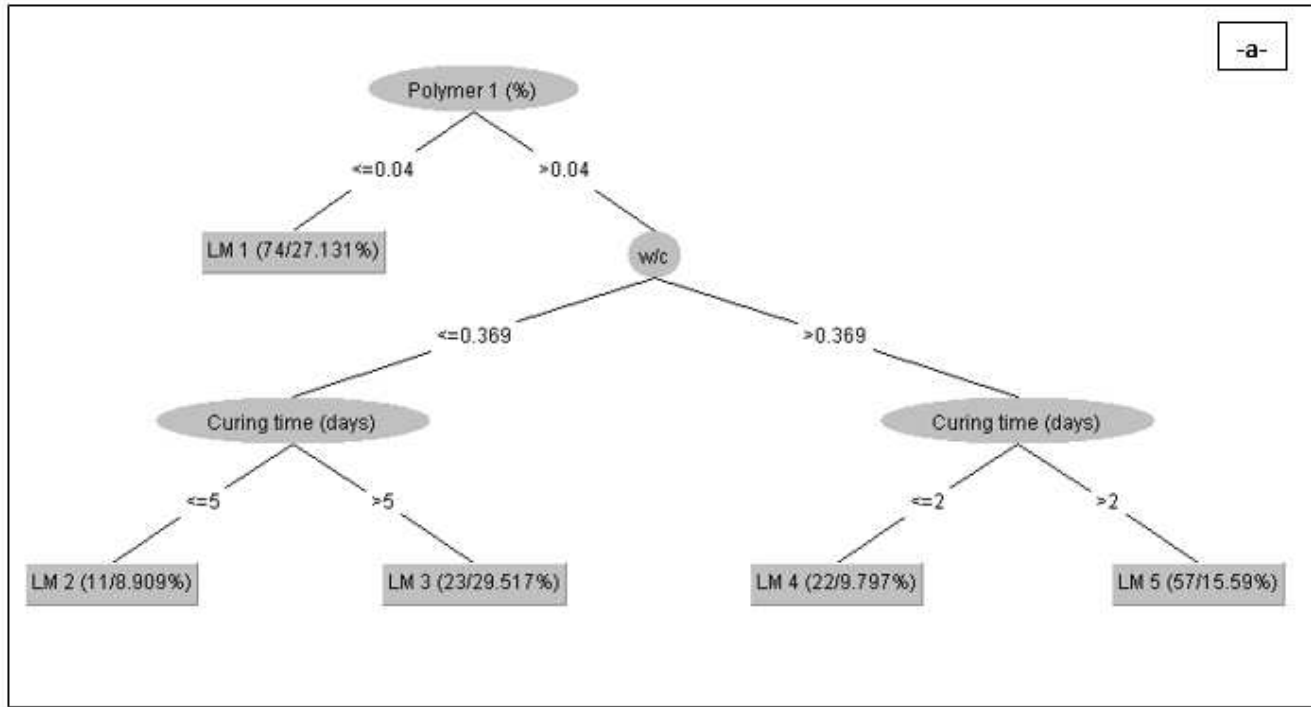


Figure 14

M5P Pruned model tree (a) cement paste modified with (a) Polymer 1 and (b) cement paste modified with

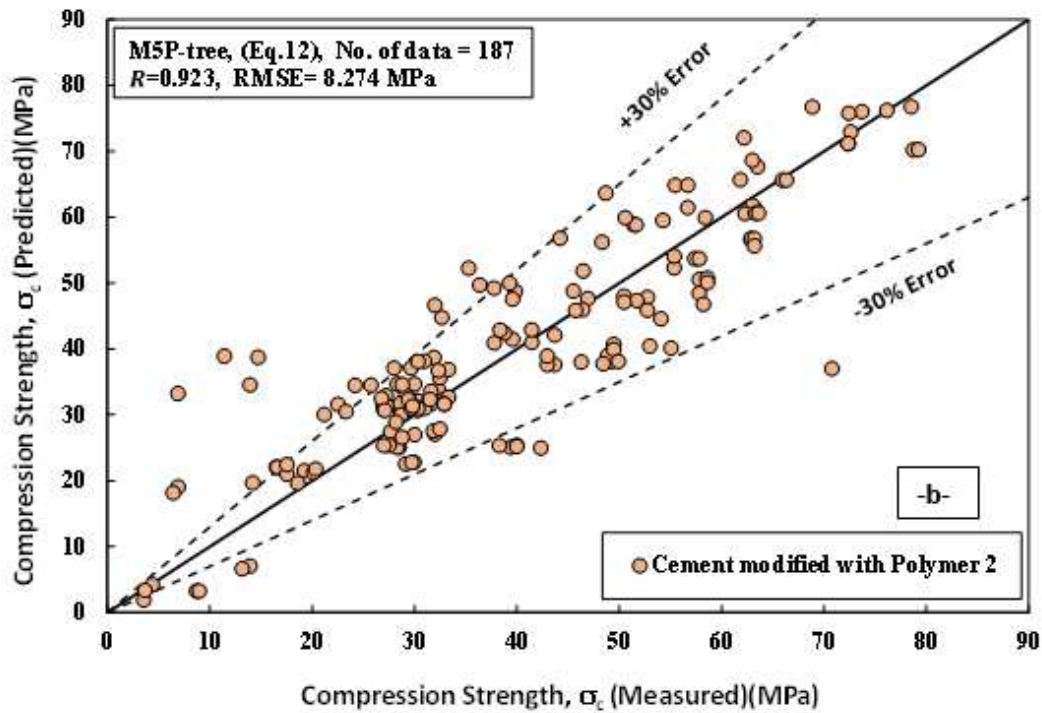
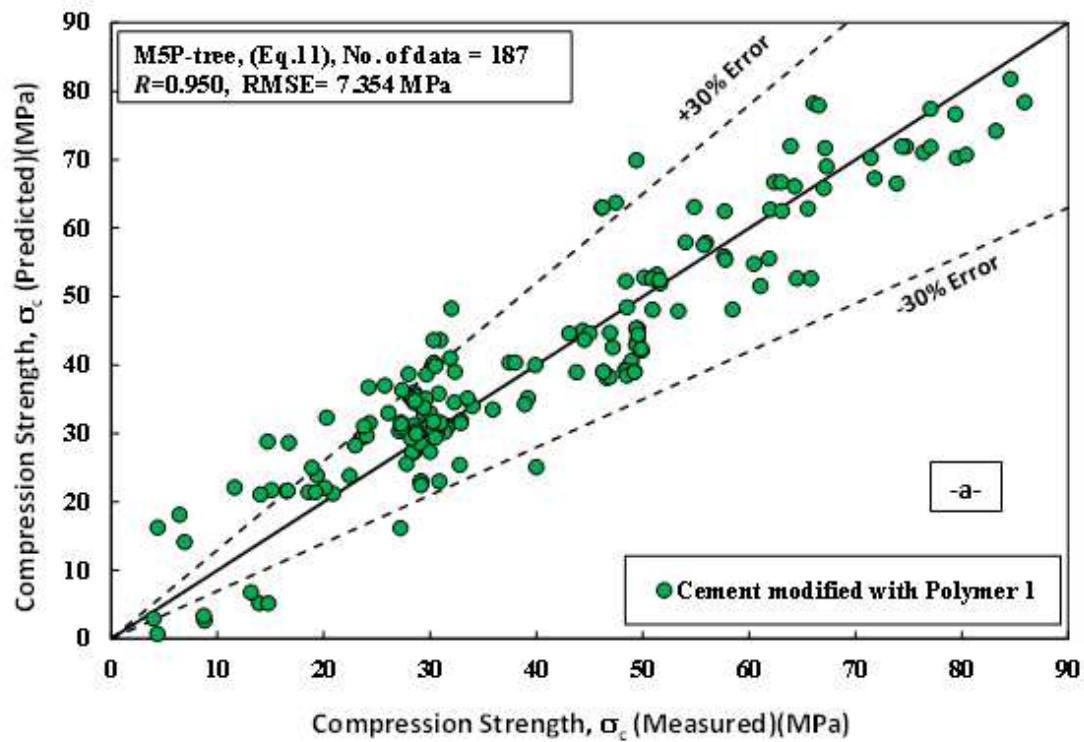


Figure 15

Comparison between measured and predicted the compressive strength of cement paste modified with polymers using M5P-tree Model (M5P) for the training data (a) polymer 1, and (b) polymer 2

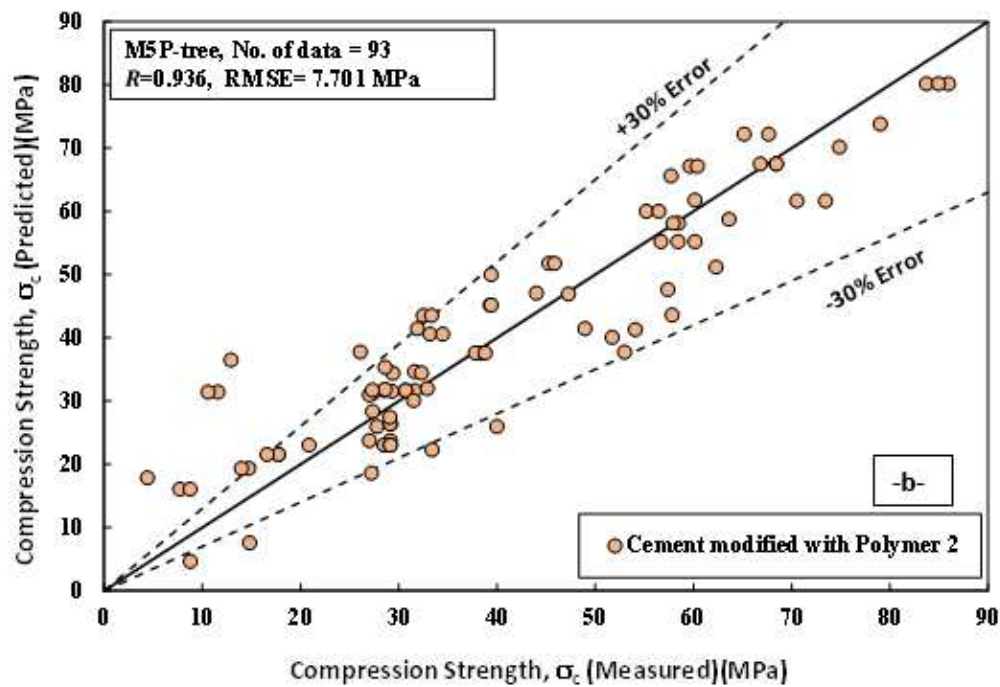
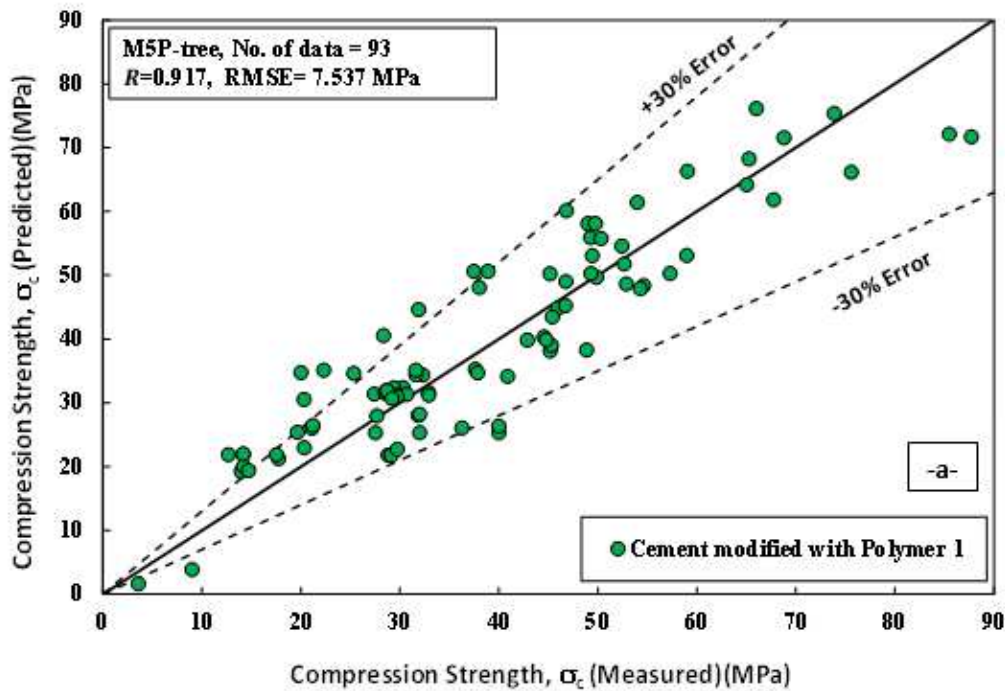


Figure 16

Comparison between measured and predicted the compressive strength of cement paste modified with polymers using M5P-tree Model (M5P) for the testing data (a) polymer 1, and (b) polymer 2

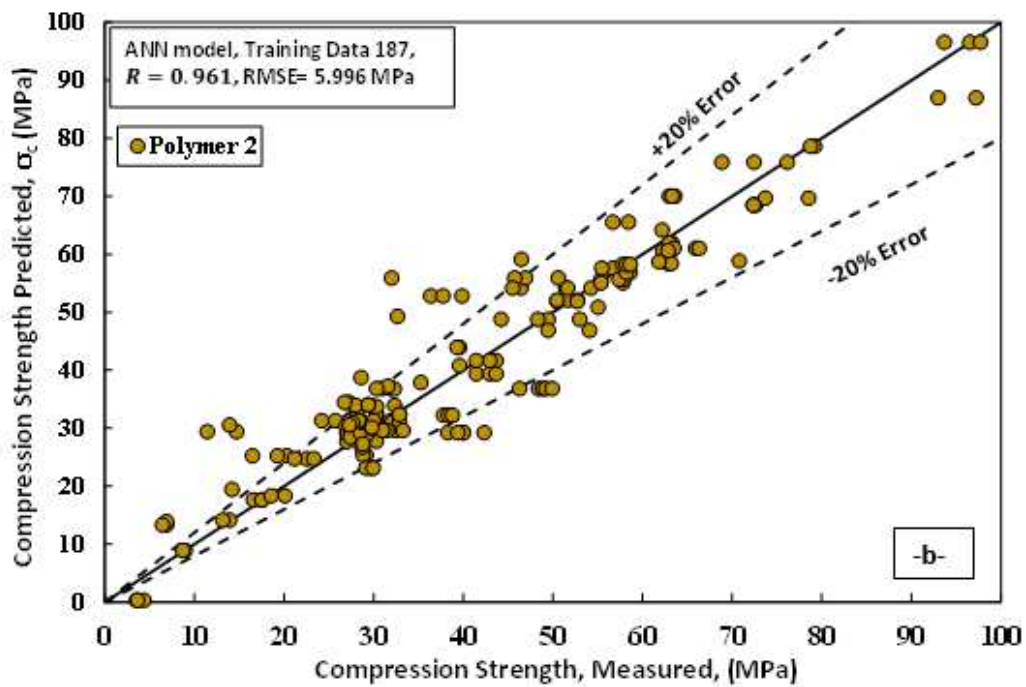
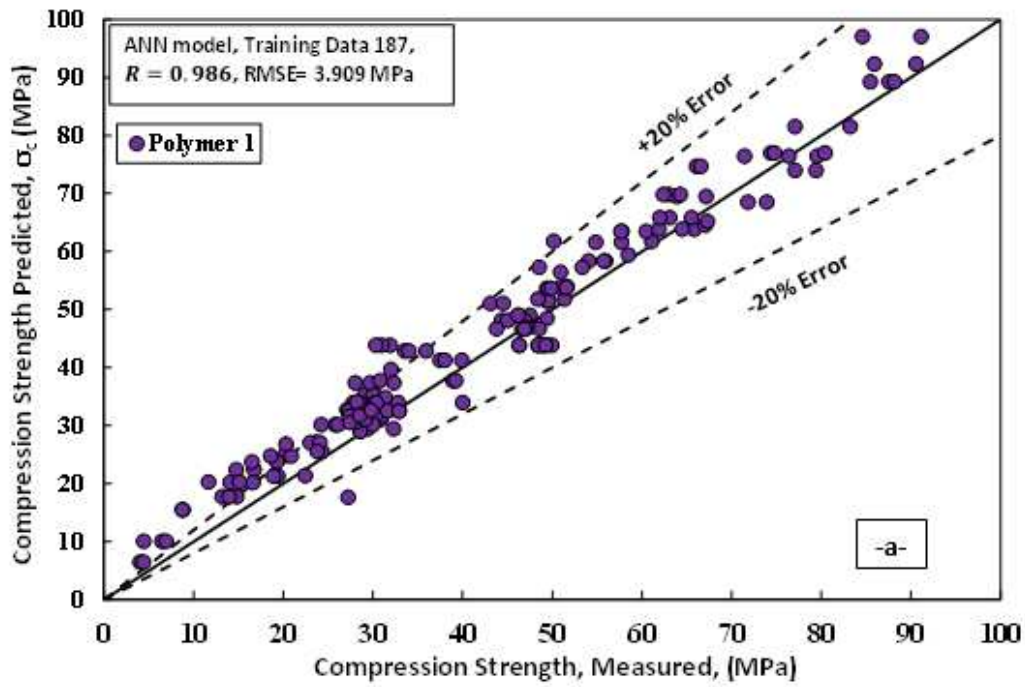


Figure 17

Comparison between measured and predicted the compressive strength of cement paste modified with polymers using ANN Model for the training data (a) polymer 1, and (b) polymer 2

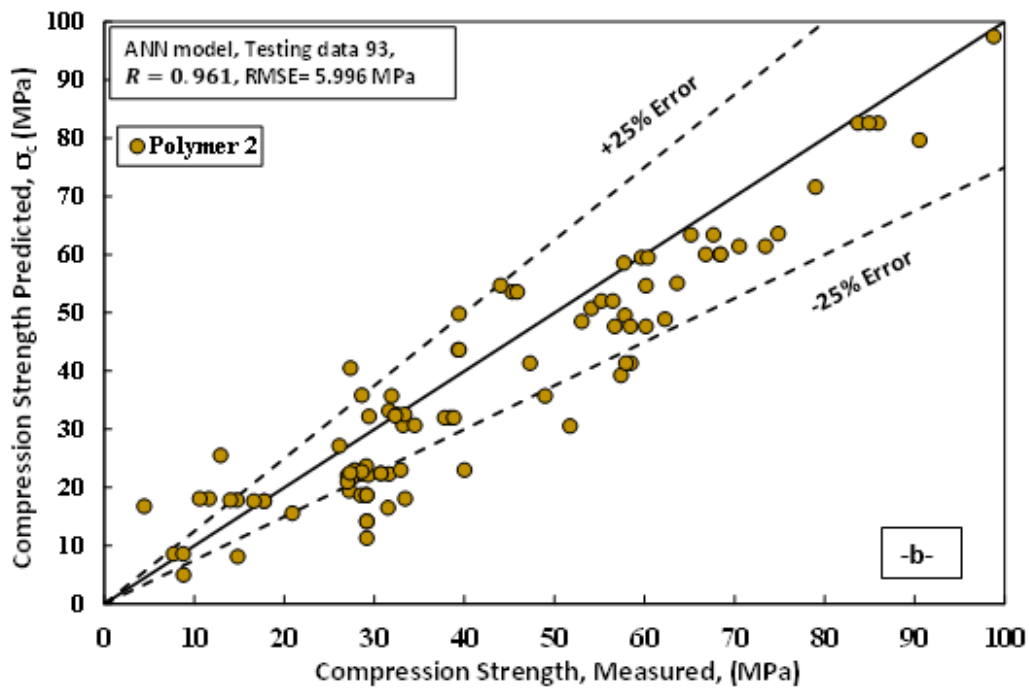
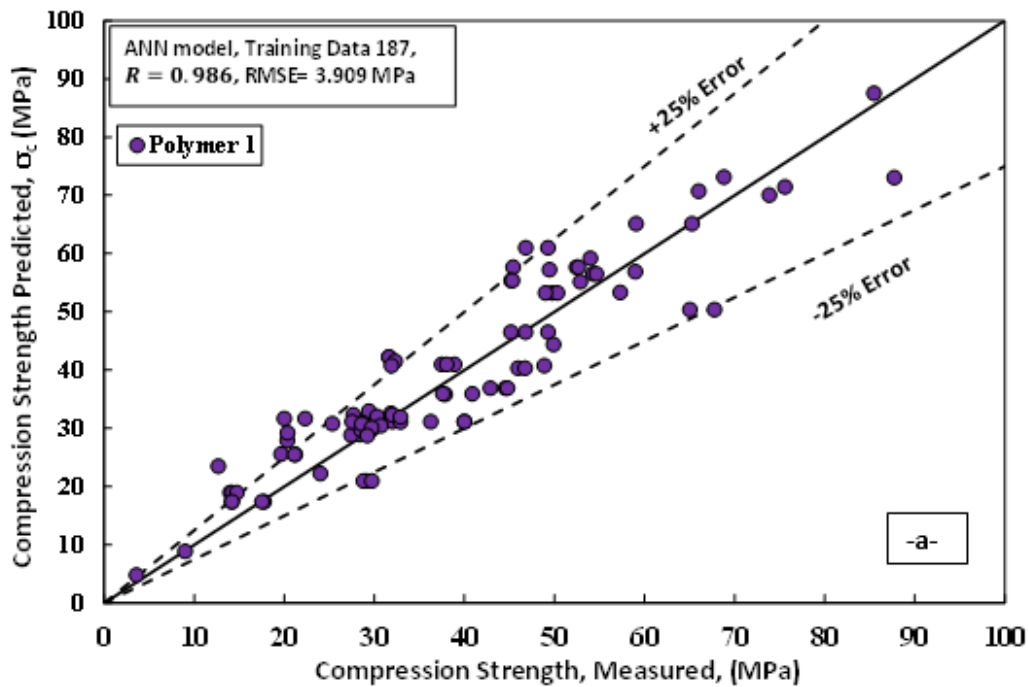


Figure 18

Comparison between measured and predicted the compressive strength of cement paste modified with polymers using ANN Model for the testing data (a) polymer 1, and (b) polymer 2

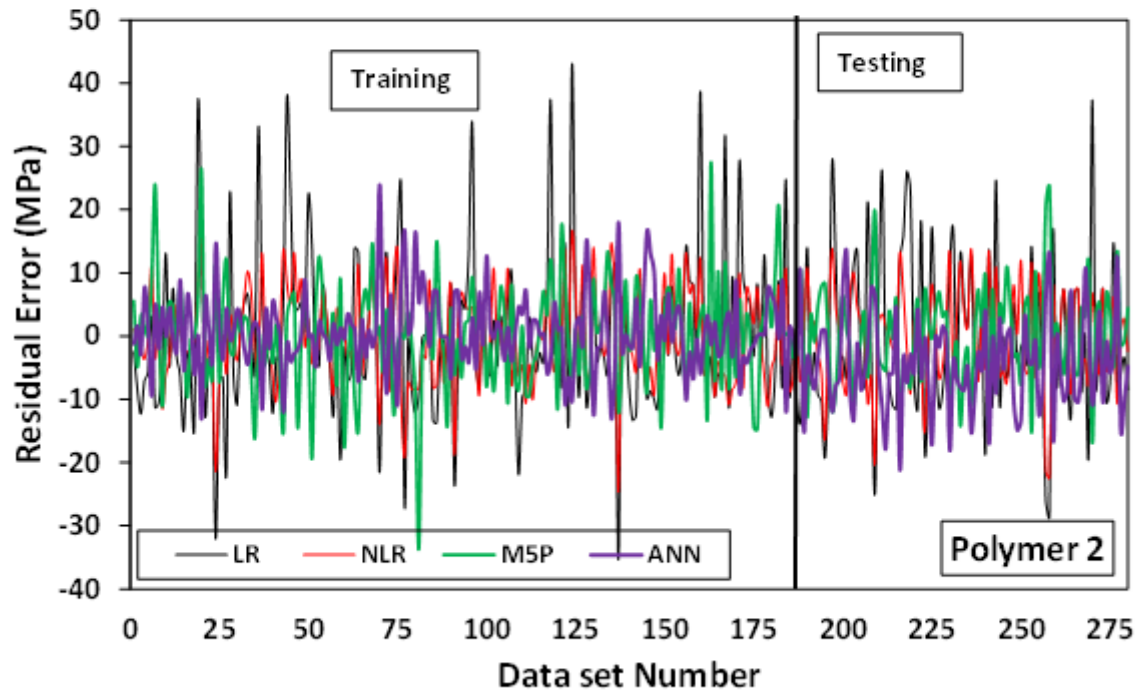
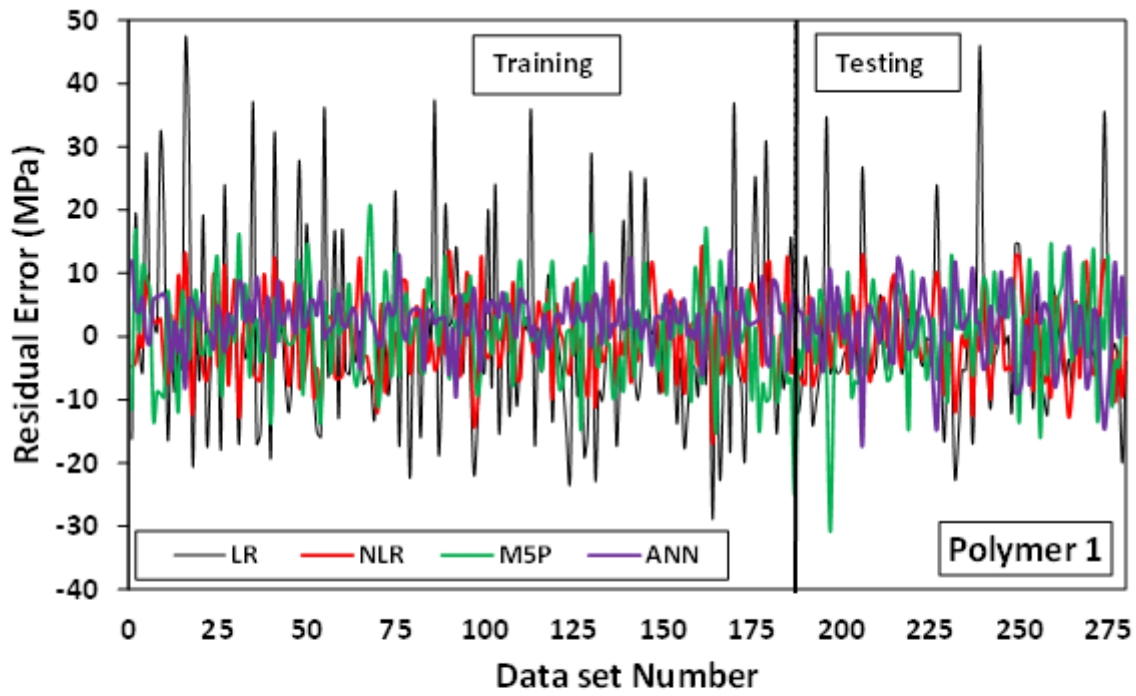


Figure 19

Variation in predicted values of compressive strength for cement paste modified with polymers based four different approaches in comparison to observed values