An Integrated Recommender System and Machine Learning-Assisted Approach to Predict Epoxy-Silica Composites' Mechanical Behaviors

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Abstract - *Machine learning (ML) approaches have been employed in the material selection step in plenty of fabrication processes of composites. Using an ML approach enables us to optimize the manufacturing process, fillers content, and additives characteristics that construct the composite structure to reach the best mechanical, thermal, chemical, and physical properties. However, the accuracy of the ML methods depends significantly on the dataset and the feature extraction methods. Therefore, filtering the dataset to remove the irrelevant data could notably assist the ML method in improving the final prediction accuracy. In this paper, inspired by the developed recommender system (RS) methods mainly used in the social network, we adopted an accurate RS model to integrate with an ML approach to predict the mechanical properties of epoxy-based composites filled with different content, size, and density of silica particles. In fact, the used RS acts as an extra filter to clean the dataset. Also, to evaluate the integrated RS and ML model, we used a regular ML model where the database is selected without having an extra filter. Eventually, the performance of the integrated RS was evaluated with the data obtained in the experiments. The results demonstrated that the prediction accuracy of the outputs variables (including compressive yield strength, impact strength, and hardness) was significantly higher for the integrated RS and ML model, comparing with the regular ML model, which was not assisted with the RS approach.*

Key Words: Machine learning; Recommender system; Epoxy composite; Silica; Mechanical properties.

1. INTRODUCTION

Composite was started to be used back to 1500 B. C; however, they have been employed as the new materials in various fields, including mechanical engineering[1-3], aerospace[4,5], civil engineering[6-8], and polymer[9-11], within last decades. The massive application of composite materials has always been inspiring for researchers to reduce their fabrication costs. One of the methods to produce low cost, but high quality, composites are predicting the mechanical properties of new ones before making them. Thanks to the recent progress in machine learning (ML) approaches, we can develop composites with optimum properties and save the final production cost and time.

One of the critical factors that limit a product's application is how it reacts against the mechanical loads. Therefore, exploring the mechanical properties of a product made from composite materials can improve its usability. The mechanical properties determination of composite has been investigated within the last decades. However, producing a new composite requires enormous investment and is also time-consuming. Moreover, the obscure outcome increases the risk of making a newly generated composite because its properties might be undesired. Therefore, predicting the mechanical properties of new materials using prediction systems methods, like ML, significantly improves the production efficiency.

Recently, many publications containing mechanical properties have been published by enormous publishers in the composite research area; however, the researchers who want to use those data have always raised a question: "how much the data are trustable?". It is straightforward that using a questionable database in a prediction material system can disturb the whole composite production project and even reverse the properties of the designed material. Therefore, it is necessary to find the correct data set prior to starting the ML process. The confirmed data set can be employed in an ML system to predict the composites' behaviors in the next step.

One of the main commonly used and well-developed methods in predicting the customers' preference to choose an item or a service is using a recommender system. The appearance of internet shopping and services, and subsequently the unprecedented rate of online users, has also helped recommender systems to be highly developed. The rich database generated by recommender systems from the users' social network activity inspires researchers to employ them in the other fields as a critical element for objects' rating and filtering. As a result, utilizing an accurate recommender system that has been used and testified successfully could be a reliable approach in rating publication, filtering the questionable ones, and eventually predicting trustable data set to be employed in an ML process.

This paper aimed to predict the mechanical properties of an epoxy-based composite. Epoxy resin has been used as the matrix for various composites that have coating applications, including coating colors, flame retardant coatings, and damage resistance coatings[12-14]. To improve the thermal and mechanical behavior of the epoxy resin, it needs to be combined with some supportive fillers. One of the well-known fillers that have been shown good compatibility with epoxy is silica particle[15-17]. Here, we developed a novel machine learning approach that is assisted by a well-developed and tested recommender system [18] to predict the mechanical properties of the composite. Also, a non-assisted traditional machine learning approach was utilized to evaluate the performance of the integrated recommender system and machine learning model. Eventually, the data of both methods were compared with the results obtained by experiments. The results demonstrated that combining a recommender system with machine learning could significantly improve prediction accuracy.

2. Material and method

In this study, to the best of our knowledge, an integrated recommender system and machine learning (RS-ML) approach for the first time was developed to predict the mechanical properties of an epoxy-based composited filled with silica particles. To evaluate the RS-ML process, another method was employed, in which a traditional machine learning technique was used for the outputs' prediction. In the first approach, 20 papers selected by the RS method were used as the experimental data set. Then, the RS-selected data were imported to an MLR method to obtain the predicted properties. In contrast, in the second approach, 20 papers were randomly chosen (out of 112 related papers found on the google scholar website) to be used as the source of data for the MLR method. Eventually, the validation of the two approaches was evaluated by comparing the experimental data obtained from lab-fabricated composites and the data received from the MLR of the two approaches.

2.1 Material

Diglycidyl-ether bisphenol A (Epikote 828) resin, supplied from Dow Chemical Company, was used as the matrix, and the hardener was chosen as DEH 24 (same supplier). Silica particles with various densities were purchased from Cabot Corporation.

2.2 Preparation

Experimental samples were prepared through a solution processing method (Gupta, 2008). The viscosity of the matrix was reduced by heating the epoxy matrix up to 50 °C. Then, the matrix was filled with silica particles of different contents. A magnetic mixer followed by a mechanical blender (1500 RPM working speed) was employed to disperse the particle homogeneously through the matrix. After degaussing the mixture with a vacuum (60 minutes), the hardener (with a 15:1 weight ratio) was added to the matrix and blended for 5 minutes. The final mix was poured inside the models and left at room temperature for curing.

2.3 Characterization

The compressive strength of the samples was measured by an ADMET compression machine (made of USA) using ASTM D6950 standard. The compression rate was 2 mm/min, and the test was finished once the sample was crippled. To evaluate the impact strength of specimens, a notched Izod impact test was performed. The impact machine was ZWICK, and ASTM D256 was utilized as the standard.

2.4 Data Collection

To collect the most relevant data to our composite's structure, we searched google scholar and selected 246 papers from the recently published publications (since 2010 to 2020). In the next step, 102 articles were excluded from our data set since their title did not contain one of "epoxy", "silica", and "mechanical properties" keywords. Eventually, 112 papers were included in our database after reading their abstract comprehensively. Next, the most important variable determining the mechanical properties of silica-epoxy composites were selected, weight fraction percentage of silica particles (wt. %), the particles' size, and the particles' density. At the final stage, these variables' information was extracted from the articles and categorized to be used in the machine learning method.

2.5 Feature Extraction

The first step of an RS procedure is feature extraction. For all of the 112 selected articles, the following meta-data were extracted. First, the quality of journals: the papers were ranked according to the journals that published them (rated from Q1 to Q4). Second, the number of authors: the number of authors contributing to the work was extracted. Third, the authors' affiliations: this criterion categorized the paper based on the authors' affiliations according to the "www.topuniversities.com" website.

2.6 Recommender System method

There are a plethora of studies on recommender systems and their improvement [19-21]. In this study, we selected a method based on the collaborative filtering method[22-24]. This type of RS is based solely on the past interactions recorded between users and items in order to produce new recommendations. We also desired to consider the relations between publications and their authors to select the most informative studies, which correlate our approach to a social recommender system[25,26]. To this aim, we selected an accurate social recommender system with high precision recommendations [18]. Ebrahimi et al. [18] introduced a social recommender system that produces recommendations with high accuracy. In our study, the publications with the most informative authors and content were selected using the mentioned social recommender system. To follow[18], we generated a social network (SN) for the selected publications based on authors' affiliation. Therefore, each publication is a node, and those publications with authors with the same affiliations have a link in this network. This network, along with the features extracted earlier, was fed into the social recommender system. As a result of the RS, the top 20 most informative publications were selected for the remainder of our analysis.

2.7 Machine learning method

Thanks to new advances in material science and numerical modeling in recent decades, simulations can predict the materials' properties before even experimentally measuring them. Applying these simulation models has significantly decreased the fabrication costs and time due to eliminating synthesis and testing steps for unfavorable materials[27]. Nowadays, various machine learning (ML) approaches have been developed that employ artificial intelligence to compute output variables based on the large datasets generated experimentally[27,28]. ML algorithms are able to discover hidden patterns just from the portion of possible data and consequently relate a target variable to a group of input variables within the best mapping way[29].

Numerous ML approaches have been introduced applicable for various purposes, including linear regression, artificial neural networks (ANNs), and logistic regression[30]; however, Among all these algorithms, linear regression (considered as supervised learning) has been studied more profoundly well-liked for its simplicity[31]. Multiple linear regression (MLR) is a type of LR that predicts the value of a dependent variable with several independent variables using a linear model[27]. The logic of the MLR approach is based on minimizing the sum of square error values between observed and predicted amounts. Equation 1 shows the general form of an MLR method:

$$Y = \alpha_0 + \alpha_1 X_1 + \cdots + \alpha_n X_n + \varepsilon \qquad (1)$$

where Y, α_i, X_i, and ε stand for the dependent variable, predicted constraints, independent variables, and error value.

3. Results and discussion

Previous studies have demonstrated that silica particles can be used to elevate the mechanical properties of thermoplastics[32-34]. Riahipour et al. [13,35] also showed that the ultralight silica aerogel particles could significantly improve the mechanical and thermomechanical properties of the epoxy-based composites used as the coatings attributed to their extraordinary properties (including high specific area and low density). Inspiring to the studies mentioned above, we employed both ultralight silica aerogels (with 0.05 g/cm^3 density) and the regular weight silica particles (with 1 g/cm^3 density) to improve the mechanical properties of the composites made from an epoxy resin as the matrix.

To find the best composites with higher mechanical properties, three main characteristics of any composites (including the filling content, the density of the filler, and the fillers' particle size) were opted. Using a well-developed method[36], the practical values of these characteristics were extracted from the trustable previously published papers studies to be entered in a machine learning process as the inputs. After finding the predicted values of input variables, we compared them with the composites made in the laboratory conditions.

Two approaches were utilized to determine the data set used as the source of MLR. In the first approach, called integrated RS-MLR, the top 20 most informative publications were selected based on the RS filtering method. We Also developed another model (called single MLR) to compare with integrated RS-MLR and evaluate the performance of applying recommender systems. In the single MLR model, in order to select the informative publications, we separated another dataset of 20 publications (equal to the number of publications recommended by our applied recommender system method). These 20 publications were randomly selected from the 112 included papers. Therefore, for evaluation, we have two different datasets: a) RS data, b) random data. Fig 1 shows the flow of two approaches in a flow chart format.

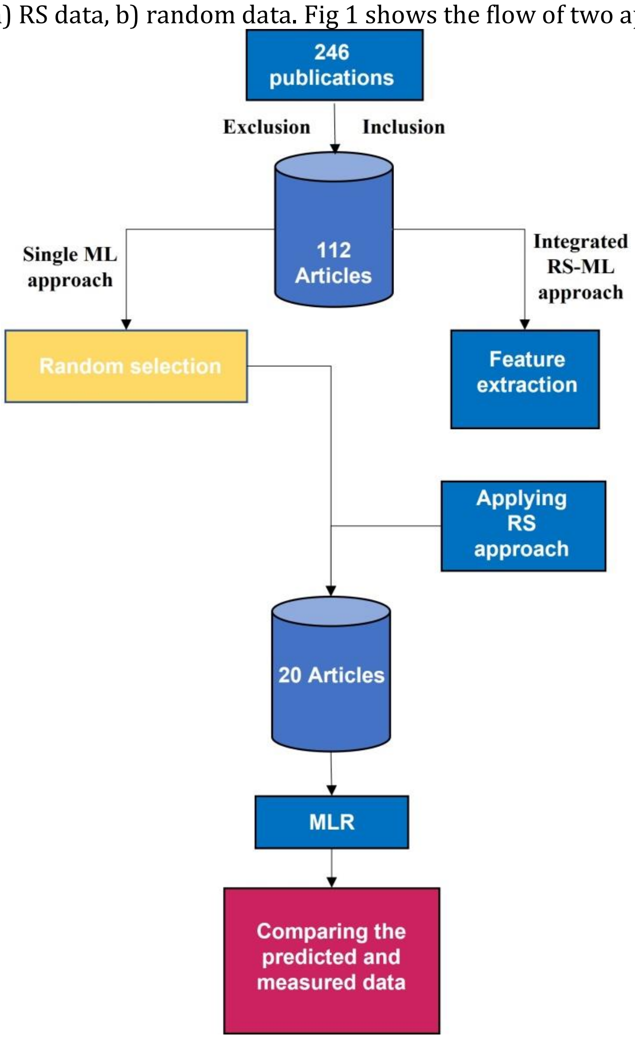

Fig -1: A flow chart showing the RS-MLR and single MLR procedure.

Tables 1 and 2 exhibit the input variables of MLR and also the mechanical characteristics of the epoxy-based composite (including compressive yield strength, impact strength, and hardness) that were predicted by the integrated RS-MLR and single MLR models, respectively. The weight fractions, particle sizes, and density were selected as the best ones reported previously[32,35,37].

A multilinear regression (MLR) was used as the machine learning model for predicting the outputs. Due to the simplicity and high interpretability of the MLR approach, it has been employed in a variety of composites research studies so far[27]. In addition to the compressive strength of concrete[38,39] and heat-treated wood[29], the MLR approach has been employed to determine the hardness[40] and impact strength[41] of materials and composites. In the MLR approach, the predictors (independent variables) estimate the predictand (dependent variable) value based on minimizing the sum least-squares of differences between observed and predicted values. In the next step, after determining the models' error function, the input weights were calculated through an optimization algorithm (Adam optimization[42]). The following equations show the predicted outcomes of two models. First, for the integrated RS-MLR model:

$$CYS = 53.0 - 2.34X_1 - 1.67X_2 + 2.35X_3 \quad (2)$$

$$IS = 12.54 + 1.11X_1 + 2.89X_2 + 5.05X_3 \quad (3)$$

$$HA = -13.00 + 4.05X_1 - 1.22X_2 + 1.54\, X_3 \quad (4)$$

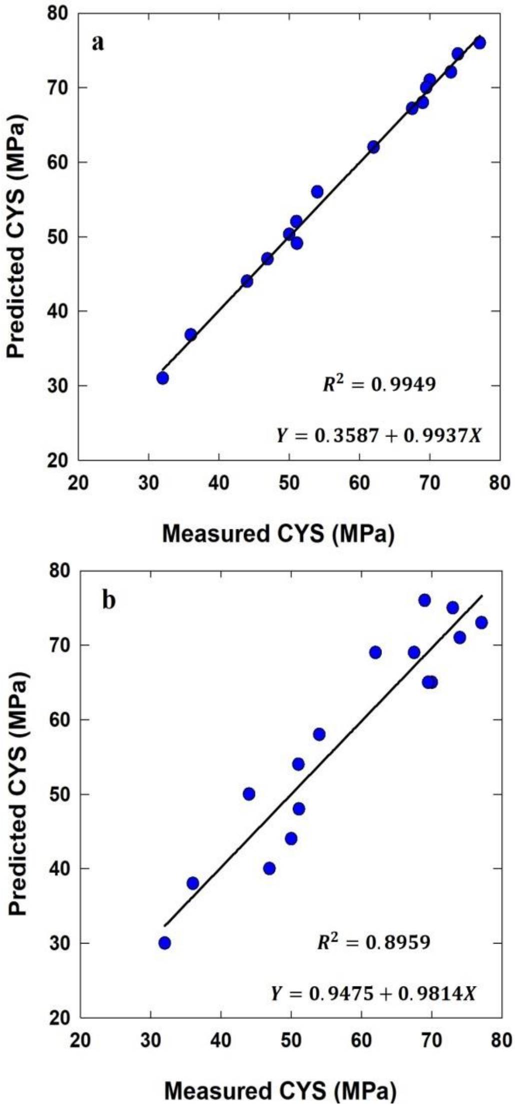

Fig -2: Measured and predicted values' relationships for CYS. (a) predicted values were obtained from the integrated RS-MLR model. (b) predicted values were obtained from the single MLR model.

Table -1: The predicted mechanical properties of the samples from the integrated RS-MLR model.

Wt. (%)	Particle size (μm)	Density of Silica (g/cm³)	Predicted compressive yield strength (MPa)	Predicted impact strength (Kj/m²)	Predicted hardness (Hv)
0.5	5	0.05	76	11.2	14.9
1	5	0.05	71	12.5	16
2	5	0.05	68	10	17.2
4	5	0.05	62	8.8	15.5
0.5	5	1	74.5	10.5	13.6
1	5	1	72.1	11.8	15.4
2	5	1	70	9.6	16.9
4	5	1	67.2	8.1	16
0.5	10	0.05	56	9.6	12.5
1	10	0.05	52	10.1	14.6
2	10	0.05	49.1	9.1	15.6
4	10	0.05	47	8	14.8
0.5	10	1	50.3	7.8	11.1
1	10	1	44	8.3	12.3
2	10	1	36.8	6.5	13.8
4	10	1	31	4.2	12.2

where CYS (compressive yield strength), IS (impact strength), and HA (hardness) are the dependent variables calculated with the MLR and X_1, X_2, and X_3 are the independent variables (weight fraction, particle size, and density, respectively). Also, for the single MLR model, the machine learning proposed the following equations:

$$CYS = 36.25 - 2.54X_1 - 2.31X_2 + 3.25X_3 \tag{5}$$

$$IS = 28.05 + 3.31X_1 + 2.12X_2 + 4025X_3 \tag{6}$$

$$HA = -9.00 + 1.56X_1 - 1.02X_2 + 2.11\,X_3 \tag{7}$$

To evaluate the performance of integrated RS-MLR and single MLR approaches for all compressive yield strength, impact strength, and hardness mechanical properties, R^2 values were calculated between predicted values received as the machine learning's output and the measured quantities obtained from experimental measurements. Equation 8 shows the calculation method of R^2. The higher R^2 values demonstrate more precise prediction.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(x_i - px_i)^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \tag{8}$$

where x_i is the measured values (obtained from experiments), px_i is the values predicted by RS-MLR or MLR approach, $\bar{x}$ is the mean of predicted values, and n is the total amount of data.

Fig 2 shows the association between the measured and predicted values for compressive yield strength (CYS) achieved by integrated RS-MLR or MLR approaches. For both methods, a linear fit was found between the measured and predicted values; however, the R^2 value increased significantly once an RS-MLR was performed (risen from 0.8959 to 0.9949). This apparent elevation in the amount of R^2 demonstrate a significant improvement in the composite's CYS prediction once an integrated RS-MLR was employed instead of using an unassisted machine learning approach (single MLR).

The correlation between the measured and predicted values of impact strength (IS) obtained from the integrated RS-MLR and MLR approaches has been presented in fig 3. As you can see, a similar trend with CYS was observed for IS. For both approaches, a linear fitting explains the relationship between the predicted and measured values, but the R^2 value was significantly higher in the integrated RS-MLR approach (0.9817 versus 0.7125). In other words, implementing a recommended system method prior to the machine learning approach has helped the MLR for a more precise prediction of IS property.

Table -2: The predicted mechanical properties of the samples from the single MLR model.

Wt. (%)	Particle size (μm)	Density of Silica (g/cm³)	Predicted compressive yield strength (MPa)	Predicted impact strength (Kj/m²)	Predicted hardness (Hv)
0.5	5	0.05	73	9	13.1
1	5	0.05	65	12.1	15.5
2	5	0.05	76	8	17.6
4	5	0.05	69	7.5	15.8
0.5	5	1	71	11.2	13.8
1	5	1	75	12	14.1
2	5	1	65	9.5	17.2
4	5	1	69	7	15.9
0.5	10	0.05	58	11.2	12.4
1	10	0.05	54	8.9	15
2	10	0.05	48	7.8	15.8
4	10	0.05	40	8.7	14
0.5	10	1	44	6.9	10.8
1	10	1	50	9.6	12.5
2	10	1	38	6.1	13
4	10	1	30	3.2	12

The relationship between the measured and predicted hardness values obtained from the integrated RS-MLR and MLR approaches also proposes a consistent agreement with a linear correlation (Fig 4). However, the R^2 values show that the integrated RS-MLR model can explain 95.14 % of the measured hardness values, while at a single MLR model, this percentage drops to 86.62 percent.

4. Conclusion

In this study, an MLR machine learning method was utilized to predict the compressive yield strength, impact strength, and hardness properties of epoxy-based composites filled with silica particles. For improving the prediction accuracy, a previously developed RS integrated with MLR to assist it in cleaning the data source. Twenty articles were selected from 112 related publications using two methods (RS-assisted and random selection). The accuracy of the two methods was evaluated by comparing them with the experiments. The results indicate that the compressive yield strength's accuracy increases from 89.59 to 99.40 percent once the RS aided the MLR. Also, the predicted values for the impact strength and hardness were 26.91 and 8.52 percent more accurate once the integrated RS-MLR model was employed. Therefore, we successfully demonstrated that the machine learning approaches' performance could significantly improve if combined with recommender systems as an extra data filtering step.

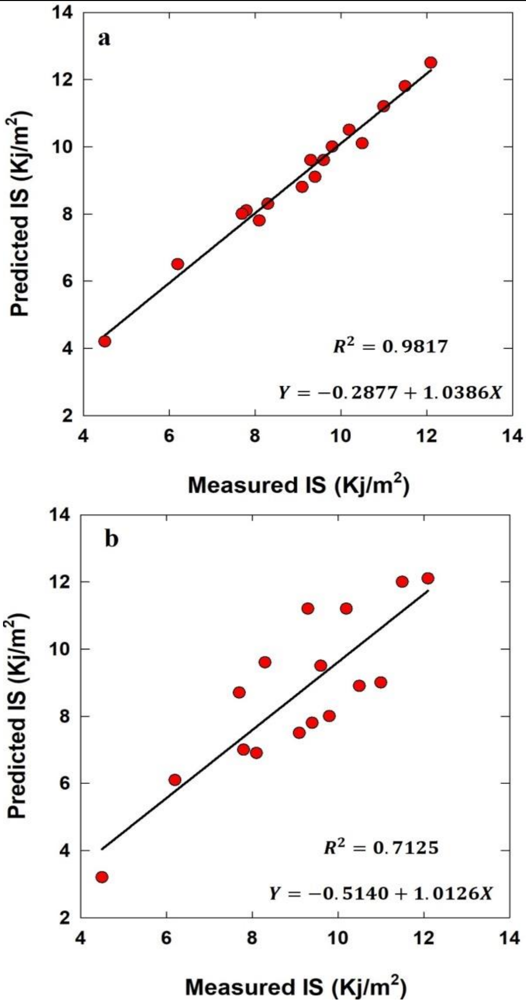

Fig -3: Measured and predicted values' relationships for IS. (a) predicted values were obtained from the integrated RS-MLR model. (b) predicted values were obtained from the single MLR model.

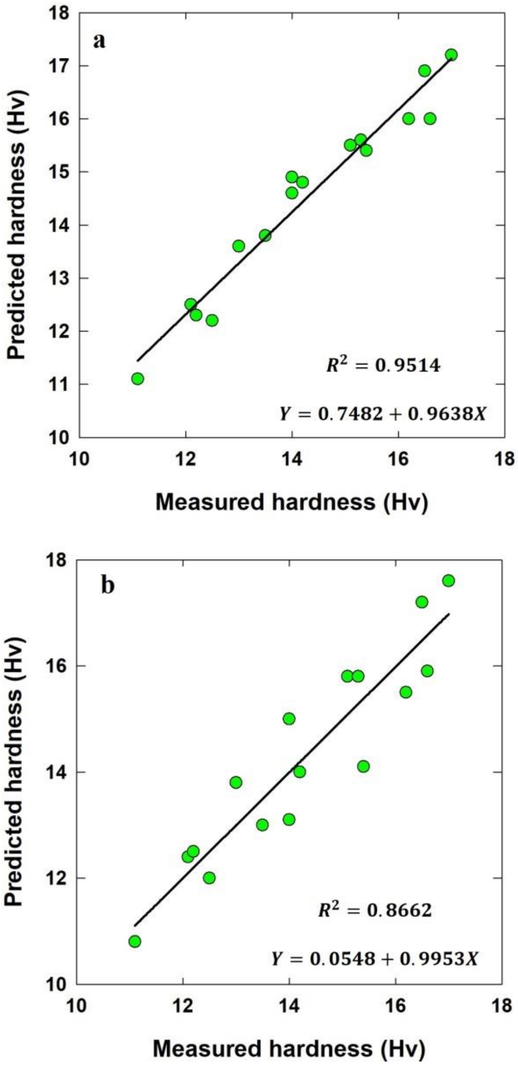

Fig -4: Measured and predicted values' relationships for hardness. (a) predicted values were obtained from the integrated RS-MLR model. (b) predicted values were obtained from the single MLR model.

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