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# Modeling constituent–property relationship of polyvinylchloride composites by neural networks

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**Abstract**

The purpose of this study is to develop an artificial neural network (ANN) model to predict and analyze the relationship between properties and process parameters of polyvinyl chloride (PVC) composites. The tensile strength, ductility, and density of PVC are modeled as a function of virgin PVC, recycled PVC, $CaCO_3$, di-2-ethylhexyl phthalate, chlorinated paraffin wax, and $CaCO_3$ particle size. The ANN model is trained using the backpropagation algorithm. The developed model was validated with a set of unseen test data. The correlation coefficient adj. $R^2$ values for test data were 0.95, 0.83, and 0.90 for tensile strength, density, and ductility, respectively. The relationship between constituents and properties of PVC composites were analyzed by sensitivity analysis, index of relative importance, and quantitative estimation. The study concluded that ANN modeling was a dependable tool for the optimization of constituents for the desired properties of PVCs.

**KEYWORDS**

artificial neural networks, index of relative importance, process variables, PVC composite's properties, sensitivity analysis

## 1 | INTRODUCTION

Polyvinyl chloride (PVC) is one of the most widely produced valuable polymers worldwide.[1] PVC is very flexible for using products that require versatile properties. The distinctive features of the PVC are due to its various constituents. The properties of PVC depend on its components such as plasticizers [di-2-ethylhexyl phthalate (DOP) and chlorinated paraffin wax (CPW)], fillers [calcium carbonate ($CaCO_3$), titanium dioxide, etc.], flame-retardants, stabilizers, coloring, and antistatic agents, as well as recycled PVC and other polymers.[2–5] The inclusion of more amount of fillers will reduce prices, but it affects the processing and weakens properties.[6,7] Recycled PVC became a highly desirable component to use as one of the constituents in PVC composite production due to availability, economic, and environmental causes.[6,8] The relationship of these multicomponent with properties is complicated and not precise until now. One way to obtain the desired PVC properties is to understand the relationships between features and their constituents. Establishing a predictive model to correlate the relationship will be highly desirable. Developing mathematical equations is difficult, hence, data-driven techniques, artificial neural networks (ANN) are handy to relate multiple inputs and outputs. ANNs were successfully used for predicting mechanical properties of medium carbon steels,[9,10] titanium alloys and deformation behavior in Ti alloys.[11,12]

The ANN models were used for various phenomena in polymer composites; compressive strength of polyester composites,[13] mechanical properties of polymers,[14–16] acoustic properties,[17] specific volumes,[18] PMMA fiber diameter,[19] clay nanocomposites[20] and to the optimization of ultrafiltration membranes.[21] Yet, there are still a couple of critical issues that need to be investigated. Altarazi et al[22] predicted properties as a function of its constituents and concluded the need for modeling the relationships between them. The purpose of this research is to develop a systematic framework to discover the connections between PVC properties and its constituents.

ANN models were developed for estimation of the relationship between properties as a function of virgin PVC, recycled PVC, $CaCO_3$, DOP, CPW, and $CaCO_3$ particle size. The objectives of the present study are

1. To predict the properties at new instances within the predictive range.
2. To estimate the relationship between properties and constituents.
3. To determine the optimum parameters for the maximum tensile strength of PVC composite.

## 2 | MATERIALS AND METHODS

The experimental data of the present work were collected from published literature.[22] The data consist of properties (tensile strength, ductility, and density) of PVC and respective constituents, that is, virgin PVC, recycled PVC, $CaCO_3$, DOP, CPW, and $CaCO_3$ mean particle size. The statistics of the data and the entire data are presented in Tables 1 and 2, respectively.

**TABLE 1** Statistics of the process variables used in the present study

| Variables | Min | Max | Mean | SD |
|---|---|---|---|---|
| Virgin PVC | 0.196 | 0.491 | 0.339 | 0.125 |
| Recycled PVC | 0 | 0.295 | 0.142 | 0.125 |
| DOP | 0.079 | 0.246 | 0.148 | 0.066 |
| $CaCO_3$ | 0.196 | 0.54 | 0.334 | 0.138 |
| CPW | 0 | 0.049 | 0.016 | 0.019 |
| $CaCO_3$ particle size | 5 | 10 | 7.5 | 2.526 |
| Tensile strength | 17.92 | 7.13 | 28.11 | 14.62 |
| Ductility | 1.93 | 3.27 | 2.35 | 3.75 |
| Density | 1.51 | 1.61 | 1.56 | 1.62 |

### 2.1 | Modeling procedure

In the present study, the ANN model training program and the graphical user interface design were written in C and Java, respectively. We trained the feedforward neural networks with the backpropagation algorithm using the sigmoid function as an activation function.[23,24] The model consists of six neurons (virgin PVC, recycled PVC, % $CaCO_3$, DOP, CPW, and $CaCO_3$ particle size) in the input layer and three neurons in the output layer (tensile strength (MPa), ductility (% El), and density) as shown in Figure 1. The model training involves adjusting the coefficients associated with each connection among the neurons until the calculated PVC composite's properties for each set of input data are near to the experimental values. To define the ideal architecture and to find the assurance of the model, the complete datasets are divided into 36 training datasets and 12 testing datasets. By varying the hyperparameters of ANN, selection of finest architecture for estimating the PVC composite's properties was achieved with the help of average error of the test data ($E_{tr}$) given as

$$E_{tr}(y) = \frac{1}{N}\sum\nolimits_{i=1}^{N}|(T_i(y) - O_i(y))| \tag{1}$$

where $E_{tr}(y)$ is the average error in prediction for output parameter $y$, $N$ is the number of datasets, $T_i(y)$ is the targeted output, and $O_i(y)$ is the output calculated. The ANN model used for the prediction of PVC composite's properties is shown in Figure 1. The ideal architecture with the two hidden layers having eight hidden neurons shows the average error value of tensile strength and ductility, 9.17 and 0.77, respectively. Once the architecture (6-8-8-2) finalized, we run the model by varying the learning rate and momentum term one by one. Finally, the optimum learning rate and momentum term of the model are obtained as 0.5 and 0.6, respectively. We got the smallest prediction errors of the tensile strength (0.91) and ductility (0.133) at 15 000 iterations.

### 2.2 | Transformation of coefficients of the ANN model

The prediction efficiency of the model depends upon the nature and magnitude of the coefficients (weights) of the ANN model. Figure 2 illustrates the values of initial and

**TABLE 2** The experimental PVC composite's properties and ANN model predicted PVC composite's for six independent variables

| S. No | VPVC | RPVC | DOP | $CaCO_3$ | CPW | $CaCO_3$ ps | TS Exp | ANN | Ductility Exp | ANN | Density Exp | Pre |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.196 | 0.295 | 0.246 | 0.246 | 0 | 5 | 7.156 | 15.987 | 3.364 | 3.354 | 1.678 | 1.71 |
| 2 | 0.491 | 0 | 0.246 | 0.196 | 0.049 | 5 | 15.36 | 16.861 | 4.558 | 4.766 | 1.812 | 1.81 |
| 3 | 0.246 | 0.295 | 0.196 | 0.196 | 0.049 | 10 | 10.25 | 15.499 | 3.886 | 3.948 | 1.758 | 1.757 |
| 4 | 0.339 | 0.143 | 0.335 | 0.165 | 0 | 5 | 26.95 | 26.655 | 3.294 | 2.901 | 1.448 | 1.447 |
| 5 | 0.491 | 0.049 | 0.196 | 0.196 | 0.049 | 10 | 20.19 | 20.835 | 5.142 | 5.114 | 1.454 | 1.454 |
| 6 | 0.491 | 0.049 | 0.196 | 0.196 | 0.049 | 5 | 36.41 | 36.506 | 4.92 | 4.811 | 1.648 | 1.647 |
| 7 | 0.196 | 0 | 0.54 | 0.246 | 0 | 5 | 2.502 | −3.706 | 3.462 | 3.362 | 1.696 | 1.695 |
| 8 | 0.491 | 0 | 0.246 | 0.246 | 0 | 5 | 11.24 | 7.52 | 3.642 | 3.758 | 1.494 | 1.493 |
| 9 | 0.196 | 0.295 | 0.393 | 0.079 | 0.02 | 10 | 12.38 | 15.501 | 3.652 | 3.808 | 1.602 | 1.601 |
| 10 | 0.491 | 0.196 | 0.196 | 0.098 | 0 | 5 | 43.24 | 42.24 | 2.42 | 2.506 | 1.62 | 1.618 |
| 11 | 0.196 | 0 | 0.54 | 0.246 | 0 | 10 | 2.19 | 1.458 | 3.216 | 3.152 | 1.798 | 1.797 |
| 12 | 0.344 | 0 | 0.54 | 0.098 | 0 | 10 | 8.35 | 8.347 | 2.522 | 3.088 | 1.66 | 1.659 |
| 13 | 0.491 | 0.049 | 0.196 | 0.246 | 0 | 5 | 12.70 | 12.958 | 3.58 | 3.448 | 1.62 | 1.622 |
| 14 | 0.196 | 0 | 0.54 | 0.196 | 0.049 | 10 | 3.458 | 6.5 | 3.222 | 2.963 | 1.684 | 1.683 |
| 15 | 0.393 | 0.295 | 0.196 | 0.079 | 0.02 | 5 | 14.44 | 15.884 | 4.358 | 3.802 | 1.864 | 1.863 |
| 16 | 0.246 | 0.295 | 0.196 | 0.246 | 0 | 10 | 10.02 | 16.418 | 1.984 | 2.9 | 1.796 | 1.795 |
| 17 | 0.196 | 0 | 0.54 | 0.196 | 0.049 | 5 | 3.676 | 2.618 | 3.186 | 3.451 | 1.78 | 1.779 |
| 18 | 0.196 | 0.147 | 0.54 | 0.098 | 0 | 5 | 12.37 | 13.057 | 2.352 | 2.855 | 1.956 | 1.956 |
| 19 | 0.196 | 0.295 | 0.246 | 0.196 | 0.049 | 10 | 30.37 | 15.293 | 4.676 | 4.184 | 1.882 | 1.881 |
| 20 | 0.196 | 0.295 | 0.246 | 0.196 | 0.049 | 5 | 10.19 | 14.204 | 5.128 | 5.082 | 1.292 | 1.292 |
| 21 | 0.491 | 0 | 0.246 | 0.246 | 0 | 10 | 6.438 | 10.627 | 3.582 | 3.875 | 1.75 | 1.749 |
| 22 | 0.339 | 0.143 | 0.335 | 0.132 | 0.033 | 5 | 17.17 | 18.818 | 3.216 | 3.463 | 1.508 | 1.508 |
| 23 | 0.491 | 0.049 | 0.196 | 0.246 | 0 | 10 | 38.90 | 38.956 | 1.21 | 1.168 | 1.602 | 1.602 |
| 24 | 0.246 | 0.295 | 0.196 | 0.246 | 0 | 5 | 25.45 | 16.103 | 3.264 | 3.223 | 1.558 | 1.706 |
| 25 | 0.393 | 0.295 | 0.196 | 0.098 | 0 | 10 | 16.13 | 19.335 | 2.336 | 2.589 | 1.868 | 1.873 |
| 26 | 0.393 | 0.295 | 0.196 | 0.079 | 0.02 | 10 | 18.13 | 16.135 | 2.444 | 3.213 | 1.592 | 1.6 |
| 27 | 0.246 | 0.295 | 0.196 | 0.196 | 0.049 | 5 | 12.52 | 14.529 | 4.406 | 4.878 | 1.828 | 1.836 |
| 28 | 0.196 | 0.147 | 0.54 | 0.079 | 0.02 | 10 | 8.39 | 8.609 | 2.668 | 2.575 | 2.07 | 2.073 |
| 29 | 0.344 | 0 | 0.54 | 0.079 | 0.02 | 5 | 9.844 | 9.476 | 3.592 | 3.115 | 1.794 | 1.804 |
| 30 | 0.491 | 0.196 | 0.196 | 0.079 | 0.02 | 10 | 15.00 | 13.659 | 4.77 | 4.707 | 1.68 | 1.692 |
| 31 | 0.393 | 0.295 | 0.196 | 0.098 | 0 | 5 | 18.18 | 16.909 | 3.472 | 3.224 | 1.658 | 1.669 |
| 32 | 0.491 | 0 | 0.393 | 0.098 | 0 | 10 | 14.84 | 13.2 | 3.868 | 3.872 | 1.588 | 1.599 |
| 33 | 0.196 | 0.295 | 0.246 | 0.246 | 0 | 10 | 15.60 | 16.382 | 3.702 | 2.964 | 1.576 | 1.759 |
| 34 | 0.491 | 0 | 0.393 | 0.079 | 0.02 | 5 | 19.18 | 20.617 | 3.42 | 3.364 | 1.646 | 1.838 |
| 35 | 0.491 | 0.196 | 0.196 | 0.098 | 0 | 10 | 50.12 | 50.767 | 0.814 | 0.792 | 1.766 | 1.351 |
| **36** | **0.344** | **0** | **0.54** | **0.079** | **0.02** | **10** | **8.036** | **8.381** | **2.616** | **2.936** | **1.798** | **1.589** |
| **37** | **0.491** | **0** | **0.393** | **0.079** | **0.02** | **10** | **20.46** | **18.817** | **2.126** | **4.25** | **1.522** | **1.532** |
| **38** | **0.196** | **0.147** | **0.54** | **0.079** | **0.02** | **5** | **16.63** | **7.859** | **2.444** | **3.186** | **1.49** | **1.5** |
| **39** | **0.196** | **0.147** | **0.54** | **0.098** | **0** | **10** | **16.13** | **13.767** | **1.074** | **2.571** | **1.528** | **1.538** |
| **40** | **0.339** | **0.143** | **0.335** | **0.165** | **0** | **10** | **16.33** | **22.156** | **3.112** | **2.762** | **1.682** | **1.694** |
| **41** | **0.196** | **0.295** | **0.393** | **0.098** | **0** | **5** | **15.82** | **15.502** | **4.164** | **3.95** | **1.872** | **1.705** |
| **42** | **0.196** | **0.295** | **0.393** | **0.079** | **0.02** | **5** | **13.94** | **14.572** | **3.186** | **4.735** | **1.792** | **1.797** |

(Continues)

**TABLE 2** (Continued)

| S. No | VPVC | RPVC | DOP | $CaCO_3$ | CPW | $CaCO_3$ ps | TS Exp | ANN | Ductility Exp | ANN | Density Exp | Pre |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 43 | 0.344 | 0 | 0.54 | 0.098 | 0 | 5 | 8.06 | 7.809 | 3.022 | 3.17 | 1.466 | 1.467 |
| 44 | 0.491 | 0 | 0.393 | 0.098 | 0 | 5 | 16.81 | 15.193 | 2.42 | 3.26 | 1.788 | 1.699 |
| 45 | 0.491 | 0 | 0.246 | 0.196 | 0.049 | 10 | 16.34 | 11.178 | 4.966 | 5.155 | 1.748 | 1.765 |
| 46 | 0.491 | 0.196 | 0.196 | 0.079 | 0.02 | 5 | 15.81 | 25.644 | 2.832 | 3.544 | 1.826 | 1.806 |
| 47 | 0.339 | 0.143 | 0.335 | 0.132 | 0.033 | 10 | 24.292 | 17.702 | 2.774 | 3.017 | 1.344 | 1.9 |
| 48 | 0.196 | 0.295 | 0.393 | 0.098 | 0 | 10 | 16.047 | 16.047 | 3.263 | 3.263 | 1.58 | 1.535 |

**36-48** datasets are designated as test data sets.

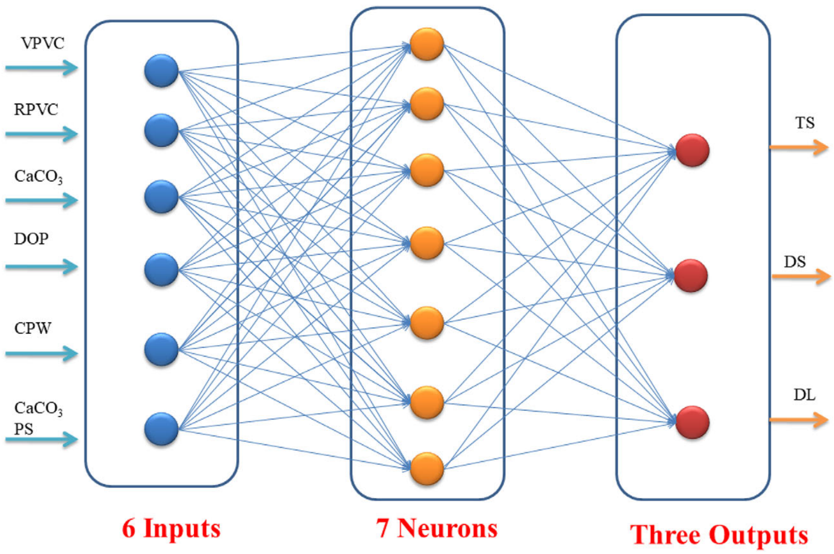


**FIGURE 1** Schematic representation of a typical multilayer feedforward network based on the backpropagation algorithm [Color figure can be viewed at wileyonlinelibrary.com]

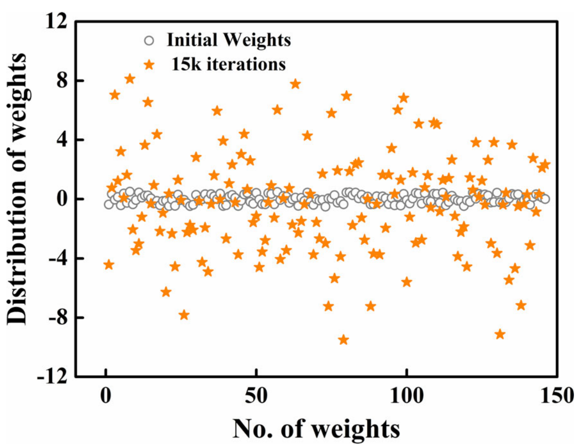


**FIGURE 2** Transformation of neural networks weights distribution as a function of iterations [Color figure can be viewed at wileyonlinelibrary.com]

optimally trained model weights. The ANN architecture, 6-8-8-2, yields a total of 146 weights $((6 + 1) \times 8 + ((8 + 1) \times 8 + ((8 + 1) \times 2 = 146)$. Initial weights were randomly generated between −0.5 and +0.5, and the optimum model values of the weights are transformed to −9.9 to +9.8, which indicates the weights within the search spaces are capable of mapping the relationship between the process parameters and properties.

## 3 | RESULTS AND DISCUSSIONS

### 3.1 | ANN model performance

The performance of the model was evaluated by predicting properties for trained and unseen experimental data. The comparison between the predicted and experimental properties was plotted as shown in Figure 3. The adjusted $R^2$ values for the tensile strength, ductility, and density are 0.95, 0.90, and 0.83, respectively, for training and testing datasets. From these correlation coefficients, we can conclude that the developed model is capable of estimating the relationship between input parameters and the PVC composite properties. Once the trained model is validated with

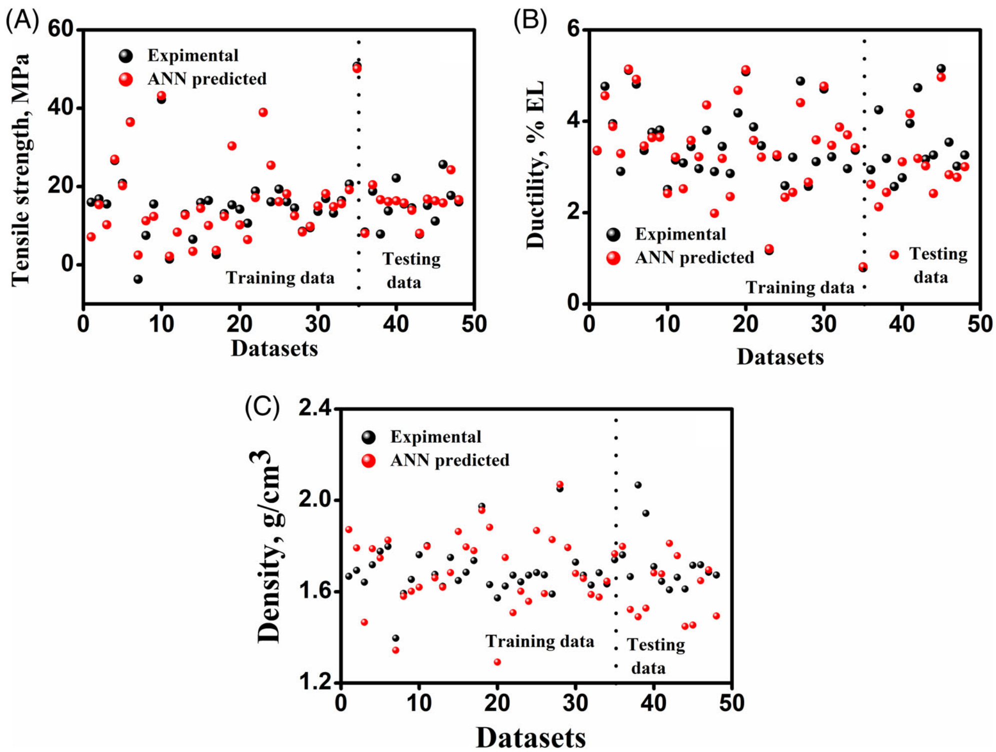


**FIGURE 3** Experimental and predicted properties: (A) tensile strength, (B) ductility, (C) density (36 training datasets and 12 testing datasets) [Color figure can be viewed at wileyonlinelibrary.com]

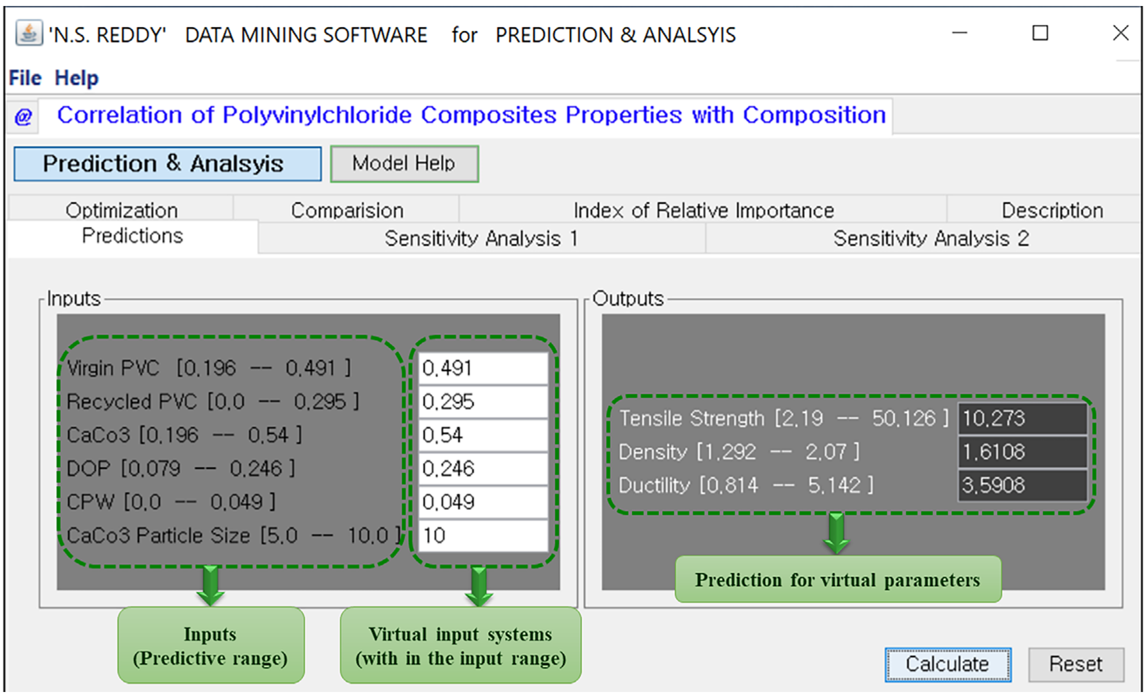


**FIGURE 4** The screenshot of the prediction of properties for the virtual PVC system [Color figure can be viewed at wileyonlinelibrary.com]

unseen data, the entire data are used to develop a model to correlate the relationship between PVC properties and the constituents. We incorporated the ANN in a graphical user interface as shown in Figure 4. Within the range of inputs, infinite combinations of experiments are possible. As the quantum of the results generated from the model is enormous, we present only a few representative ones.

## 3.2 | Influence of process parameters on PVC composites properties

### 3.2.1 | Single variable sensitivity analysis

Figure 5 shows the predicted effect of varying one input parameter on properties, keeping the remaining input

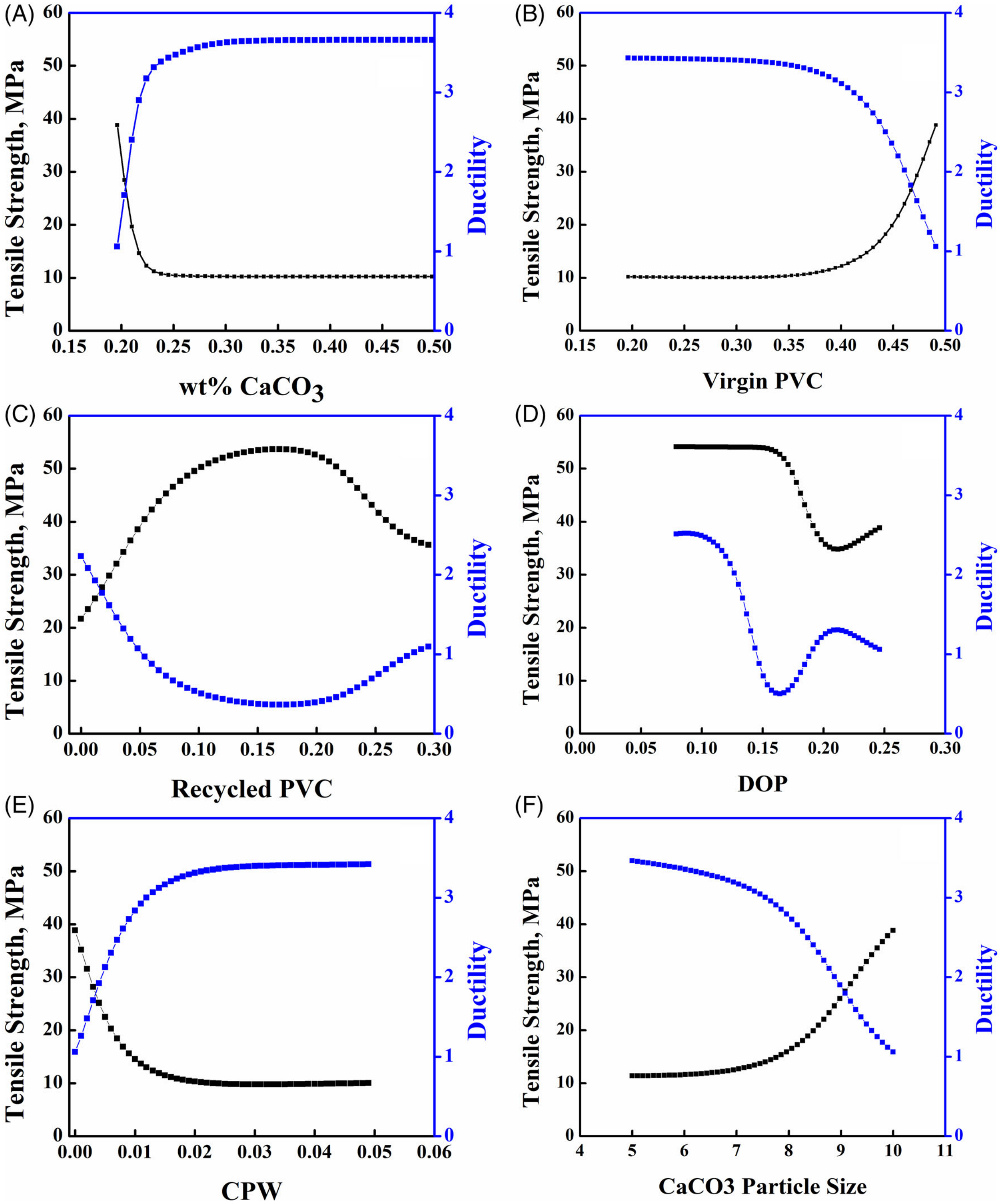


**FIGURE 5** Effect of process parameters on the PVC composite's properties: (A) wt% $CaCO_3$, (B) virgin PVC, (C) recycled PVC, (D) DOP, (E) CPW, and (F) $CaCO_3$ particle size [Color figure can be viewed at wileyonlinelibrary.com]

parameters at a constant value. Figure 5A illustrates the addition of wt% $CaCO_3$; the addition of $CaCO_3$ fillers enhances the material stiffness (the elastic modulus), whereas it reduces the tensile strength and increases the ductility.[25,26] Figure 5B shows that the tensile strength of the virgin PVC is increasing up to 50 MPa. The tensile strength depends on the type of plasticizers used; triethyl phosphate as a plasticizer will increase the tensile strength. However, in the case of ductility, it decreases with increase of virgin PVC.[20] Figure 5C shows that the recycled PVC from the bottles and pipes possesses lower tensile strength and higher elongation at break. The tensile strength will increase initially, and afterward, tensile strength will decrease because of the presence of impact modifier in the recycled PVC.[27] Figure 5D shows that plasticizers reduce the tensile strength as it weakens the bond holding the polymer molecules together, but it also facilitates processing. The DOP plasticizer will decrease the tensile strength and increase the ductility.[28]

Figure 5E shows the effect of CPW as a plasticizer; it has a weak bond holding the molecules so it will reduce the tensile strength and increase the ductility.[29] Figure 5F illustrates the increase of $CaCO_3$ particle size; the tensile strength will increase initially and then it will decrease. However, in the case of ductility, initially, it will drop and after 6.5 particle size, the ductility will increase because the brittle to ductile transition temperature was reduced confirming the toughening (able to withstand great strain without tearing or breaking) effect of the $CaCO_3$ particle size. Small contents of nanoparticles led to an increase in both elastic modulus and yield stress, although the addition of higher contents of nanoparticles did not lead to subsequent increase in these properties.[30]

### 3.2.2 | Two variable sensitivity analysis

Here, we predicted the combined effect of parameters on ductility and tensile strength. The predicted 3D surface plots for the PVC composite properties with process parameters are shown in Figure 6. Figure 6A,B shows the combined influence of recycled PVC and, in the case of an increase in recycled PVC, reduces the tensile strength because of the presence of impact modifier in the recycled PVC.[4] In the case of CPW, it has weak bonding strength between the plasticizers, not much effect on tensile strength, but in the case of ductility, it increases with increasing of CPW.

Figure 6C,D illustrates the influence of both $CaCO_3$ and DOP, in the case of increases of wt% $CaCO_3$, decreases the tensile strength. Ductility increases with increase in $CaCO_3$ fillers. In the case of DOP, there is no much effect on tensile strength. But in this case, ductility increased with increasing DOP because it weakens the bond holding polymer molecules together, but it also facilitates processing.[2]

### 3.3 | Index of relative importance ($I_{RI}$)

Here, we used the developed ANN model to calculate the index of relative importance ($I_{RI}$)[31] to identify the role of constituents on properties. The nature and magnitude of

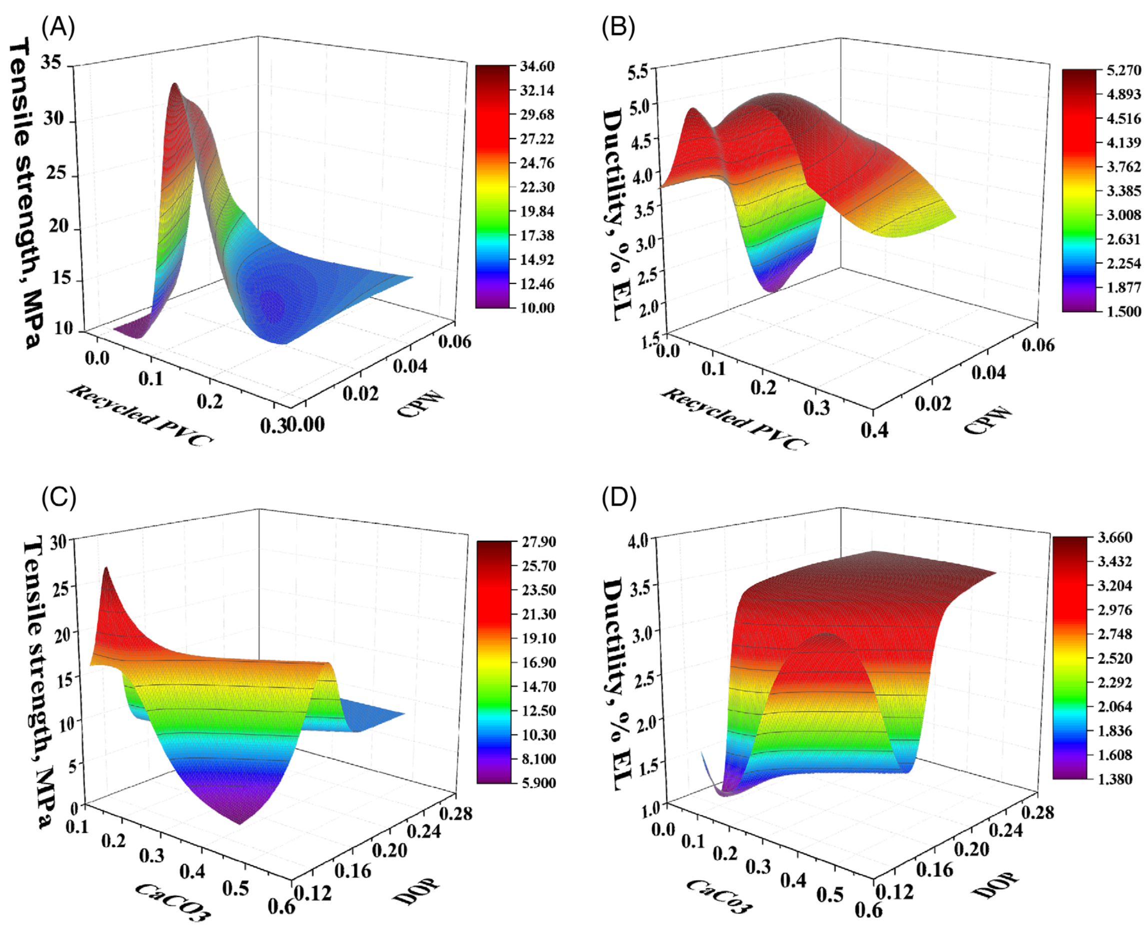


**FIGURE 6** Prediction of 3D surface plots of the effect of recycled PVC, CPW, $CaCO_3$, and DOP: (A) and (C) Tensile strength, (B) and (D) ductility when the other process parameters are constant [Color figure can be viewed at wileyonlinelibrary.com]

$I_{RI}$ indicate the significance of the input parameters on the property. All variable prominence of a system is well reported on a whole dataset.[32,33] While one input was varied with a ±5% offset, the other five inputs were kept constant. After adding ±5% variation to all the inputs, 12 combinations of input data were created. These data were fed to the ANN model (Figure 4) to predict the properties and thereby to calculate ($I_{RI}$) of each input parameter. The calculation of $I_{RI}$ was well described in the previous articles.[9]

We selected a sample number 28 shown in Table 2. We estimated the relationship. Figure 7A,B shows that the virgin PVC, recycled PVC, and $CaCO_3$ particle size are showing positive influence on tensile strength and respective negative relationship with ductility. The remaining three parameters, $CaCO_3$, DOP, and CPW, are acting negatively on tensile strength and showing positive influence on ductility. From these studies, we conclude that virgin PVC, recycled PVC, and $CaCO_3$ are more important than the other parameters. This method provided the relationship between the constituents and properties qualitatively for a particular case.

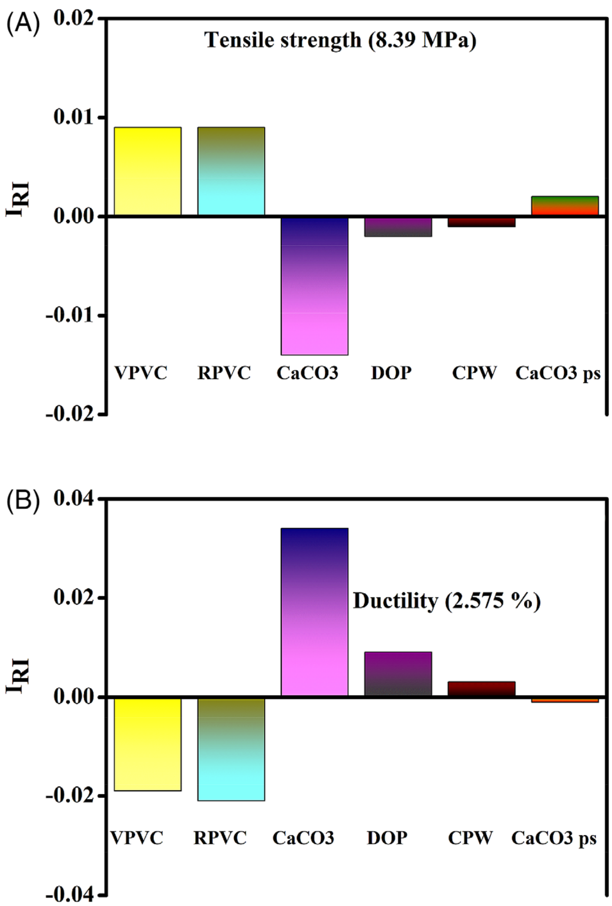


**FIGURE 7** The significance of various process parameters on tensile strength and ductility [Color figure can be viewed at wileyonlinelibrary.com]

## 3.4 | Creation of virtual PVC composites

In this section, we estimated the relationship between properties and constituents quantitatively. We calculated the average values of the database of PVC composites, and those did not exist in experimental data. By using these mean parameters, we predicted the PVC composite's properties with the help of the user interface of the model (Figure 4). The predicted values for the virtual system of the tensile strength and ductility are 28.11 and 2.35, respectively, and these values are within the values of the experimental values. We selected a sample (35 in Table 2) with the tensile strength of 50.12 and the ductility of 0.814 from the database. We changed each parameter individually to the virtual system to achieve the experimental condition of sample 35 and estimated the properties.

Table 3 shows the quantitative estimation of properties by the virtual addition of constituents. The change in virgin PVC from 0.3391 to 0.491 resulted in a marginal decrease of tensile strength and a respective increase in

**TABLE 3** The quantitative estimation of PVC composite's properties from the virtual system

| VPVC | RPVC | $CaCO_3$ | DOP | CPW | $CaCO_3$ particle size | Tensile strength | Change | ductility | Change |
|---|---|---|---|---|---|---|---|---|---|
| 0.3391 | 0.1429 | 0.3347 | 0.1487 | 0.0165 | 7.5 | 28.11 | – | 2.35 | – |
| 0.491 | 0.1429 | 0.3347 | 0.1487 | 0.0165 | 7.5 | 27.03 | −1.07 | 5.15 | 2.80 |
| 0.491 | 0.196 | 0.3347 | 0.1487 | 0.0165 | 7.5 | 18.08 | −8.95 | 5.31 | −0.16 |
| 0.491 | 0.196 | 0.196 | 0.1487 | 0.0165 | 7.5 | 42.76 | 24.67 | 4.39 | −0.92 |
| 0.491 | 0.196 | 0.196 | 0.098 | 0.0165 | 7.5 | 15.46 | −27.29 | 4.82 | 0.43 |
| 0.491 | 0.196 | 0.196 | 0.098 | 0 | 7.5 | 53.89 | 38.43 | 1.59 | −3.23 |
| 0.491 | 0.196 | 0.196 | 0.098 | 0 | 10 | 53.85 | −0.041 | 0.96 | −0.63 |
| Experimental properties for these conditions | | | | | | 50.12 | | 0.814 | |

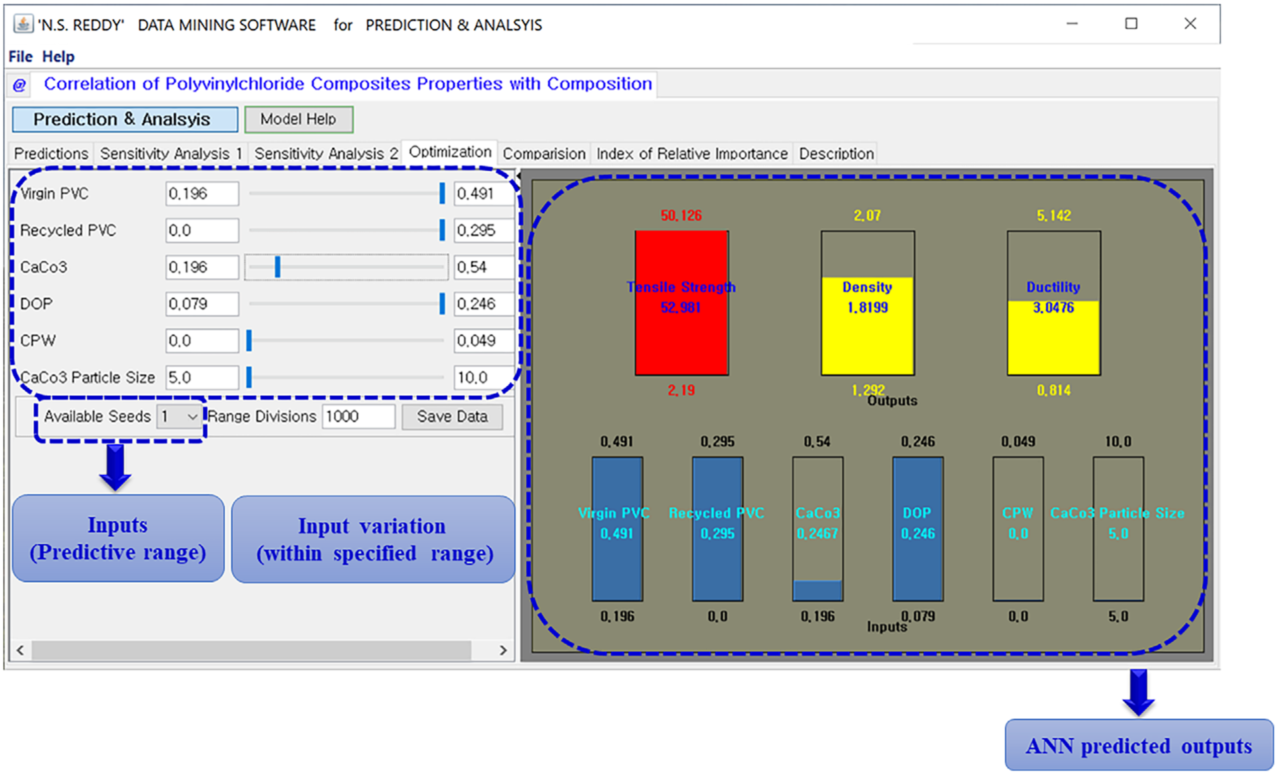


**FIGURE 8** Optimization of process variables for the maximum tensile strength [Color figure can be viewed at wileyonlinelibrary.com]

ductility and surprisingly the results are contrary to the existing knowledge.[34] An increase in recycled PVC reduces the strength and ductility as expected.[34] The decrease in $CaCO_3$ from its mean value to 0.196 resulted in a drastic increase in tensile strength and reduction in ductility. Altering the values of DOP from its mean value (0.1487) to 0.098 caused a significant rise in tensile strength and a marginal reduction in ductility and these results are in good agreement with our earlier prediction (Figure 4D).[35] Making the CPW value zero from mean values resulted in a huge increase in tensile strength and a respective significant decrease in ductility.[35] Finally, the increase in $CaCO_3$ particle size from 7.5 to 10 resulted in no change in tensile strength and a small decrease in ductility, as is expected.[36] These calculations are based on the network weights. After obtaining the experimental condition of sample 35, the tensile strength and the ductility are 50.12 and 0.814, respectively. However, the differences or controversies in the predictions, the final values of the predictions are near to the experimental values.

### 3.5 | Optimization of PVC constituents for the desired output

We developed a standalone ANN software to model the correlations between the constituents and properties, as shown in Figure 8. The proposed ANN model was able to recognize the optimal constituents of PVC composite for the desired properties. We can adjust the variables according to the desired output, as shown in Figure 8. We want to explore the possible input parameters for the maximum tensile strength and by keeping the minimum values of virgin PVC due to its high cost. We used more recycled PVC and minimum values of virgin PVC and determined the respective combinations of other constituents by using the ANN model. The highest tensile strength of 53 MPa, ductility of 3.02%, and the density of 1.82 g $cm^{-3}$ can be achieved with 0.491% virgin PVC, 0.295% recycled PVC, 0.246% $CaCO_3$, 0.246% DOP, at minimum values of CPW and $CaCO_3$ particle size. As virgin PVC is expensive, using recycled PVC is economical and environmentally friendly.

## 4 | CONCLUSIONS

In this article, we provide a systematical ANN approach for modeling the complicated relationship between PVC properties and its constituents. The developed ANN model can predict properties for an infinite combination of process parameters with reasonable accuracy. $R^2$ values for tensile strength, density, and ductility are 0.95, 0.83 and 0.90, respectively. The ANN model will be able to predict the single variable and two variable impacts on PVC composite's properties. We used the index of relative importance ($I_{RI}$) method and a virtual system to estimate the influence of each process parameter on PVC composite's properties. The proposed methods will be useful to correlate the relationship between multiple inputs and outputs. We can use the proposed model to obtain the constituents for the desired properties.

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