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Intelligent System for the Architectural Coatings Production

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Abstract

The development and production of architectural coatings is full with a lot of variables that affect the performance of the final product. Therefore, the understanding of the effects of these variables and the prediction of the properties in regular or new formulations, are critical issues for the coatings industry, since experimentation is time consuming and a lot of financial and human resources are needed to test or develop new products. In current economic conditions, cost savings and product innovation are critical issues.

In this paper, an intelligent system was developed based on an artificial neural network (ANN), of the feed forward type. This ANN was trained using as inputs key properties of titanium dioxide and two formulation parameters (pigment volume concentration and titanium dioxide content) for a water based architectural coating. The outputs of this research were spread rate, color (L, a*, b*) and tinting strength. Test data was used to check the accuracy of the model, demonstrating the viability of paint properties prediction related to the properties of the titanium dioxide formulation with high correlation (>95%).*

The intelligent system has the capability to predict, graphic and compared the properties of a set of 2 paints within a broad range of formulation parameters.

Keywords: Properties prediction; architectural coatings; titanium dioxide; artificial neural networks; paints properties.

1. Introduction

Architectural coatings are liquid pigment suspensions designed to protect and decorate houses and buildings. This type of coatings or paints could be water or solvent based and are easily applied by mechanical devices (roll, brush and spray). In Mexico, this segment represents an estimated 56% of the total production from a market of two billions dollars annually [1].

The architectural coatings industry is continuously searching for new alternatives to improve their products, by reducing costs or improving performance. However, this search in most cases is expensive and time consuming, considering the vast range of potential raw materials and the interactions among them [2].

One of the most important raw materials for architectural coatings is a white pigment -- titanium dioxide --which provides opacity, whiteness and durability to the product. For this reason, the knowledge of the performance of different grades of this pigment at different concentrations and the interaction with other components in the formulation is very important.

Property prediction for architectural coatings has been explored in a previous work, using linear regression models, with high correlation ($R^2 = 0.99$) in very restricted systems (one input and one output at a time) [3]. Other researchers, like Werner, explored property prediction for coatings, studying the particle size distribution of fillers, and finding a close relationship between narrow and broad particle size distributions with the final coatings properties like opacity, dispersion, gloss and drying time [4]. Polyakova and the Chicago Society for Coatings Technology Technical Committee considered other variables, like pigments characterization, chemical composition or substrate nature, in two studies. It was shown that correlations could be found and can explain the observed phenomenon obtained in the lab tests. The study of Polyakova demonstrated that better coating adhesion could be found changing the crosslinker concentration (not larger than 10%), and also predict the flow out and a decrease of the gelation time. The study presented by the Chicago

Society for Coatings Technology Technical Committee showed that the morphology of the pigment particle (rhombohedral and spheroidal) affect the rheology of the paint as well as gloss mainly at 20° and 60° [5, 6].

However, this type of approach does not consider the real multivariate nature of architectural coating systems, because of all the nonlinear interactions between its components.

A systematic framework is needed that allows the coatings researcher to reduce the time for experimentation while also considering more variables in their laboratory work. The development of an inferential model that reduces time and economic losses will significantly improve the performance of the companies developing these products. The selected model combines statistical analysis with artificial intelligence [7].

Artificial intelligence can be defined as information processing by mechanical devices. These devices aim to replicate the functions of real biological neurons with a few simple mathematical concepts implemented on digital computers. Artificial neural networks (ANNs) are massive interconnected networks of simple computing elements (artificial neurons) which are intended to perform an analog operation or transformation of the input signals [8].

The use of an advanced technology like artificial neural networks could assist industry in exploring the different options in raw materials and formulations required to obtain products with favorable properties or characteristics, accelerating new product launches. Some researchers, including Vitela, demonstrated the feasibility of using ANN to predict gloss and dry time on alkyd coatings, with 90% or more accuracy [2]. Also, Nascimento demonstrated a high correlation for particle size determination by laser diffraction in a highly concentrated suspension of particles in fluids [9]. This showed that the ANN could be adapted by training, and although the concentration of the fluid changed, good measurement of the particle size was maintained.

The purpose of creating an application for the coatings industry using ANN is to generate a solution that allows the technicians to reduce laboratory time, with a reliable tool that could be apply to a common formulation space. Although, neural networks can only works well close to its training space, the adequate selection of a broad variables range (through different qualities and raw material types and concentrations), could allow to use the tool broadly in the most usual paint qualities.

Therefore, the use of ANN can allow the researcher or formulator to have a high degree of confidence in their work and reduce the experimentation time.

2. Review of Neural Networks Theory

Since the ancient Greeks, the explanation of how the brain works and the thinking process were matters of study. Biological and psychological approaches were the first attempts to understand the interactions between neurons and the processes involved in the control of systems in living organisms. With the understanding of the structure of the brain and neuron connectivity, simple mathematical models were developed in analogy to biological learning. In 1943, W. S. McCulloch and W. A. Pitts presented the fundamental basis of neural computing [10].

An artificial neural network consists of multiple processing units (artificial neurons or nodes), interconnected to each other, capable of performing rapid operations for data processing in a parallel manner. These nodes are analogous to real brain neurons. The artificial nodes are connected by numerical weights, just as the real neurons are connected by synapses. Signals can travel both in series and in parallel. Later, models of adaptive stimulus response were elaborated by Farley and Clark (1954), Rosenblatt (1958), Widrow and Hoff (1960), Caianiello (1961) and Steinbuch (1961). This was the basis for the implementation of modern neural computers, which are used in a broad range of applications like pattern recognition, optimization computation, and robot control and decision support [11].

The practical first application for the neural networks, called the Perceptron, was proposed by Rosenblatt in 1958. It describes how “n” inputs are received from external *stimuli* in the environment and transmit these signals through a threshold [10, 12]. When the net input (Eq. 1) exceeds the value of the threshold or bias “b”, the output “Out” of the next layer, is activated, as shown in Eq. 2. This applies to feed forward networks, in which all links are unidirectional and there are not interconnections within the same layer [12].

$$Net_j = \sum_{i=1}^{n} w_{ji} In_i + b_j \quad \text{.....Eq. 1}$$

Here j is the label of the node and *i* is the label of the weight from input In_i. The output Out_j of the artificial neuron is the binary variable given in Eq. 2. It is 1 if the weighted sum Net_j is positive and 0 if it is negative.

$$Out_j = \begin{cases} 1 \text{ if } Net_j >= 0 \\ 0 \text{ if } Net_j < 0 \end{cases} \quad \text{.....Eq. 2}$$

While the Perceptron has some positive characteristics, including a simple iterative algorithm to determine the connection weights, it is severely limited as a computational engine. Since it has just a single layer implementing a simple weighted sum of inputs, followed by a binary decision for each node j, it can at best generate a *linear* decision surface. It cannot solve even simple problems like the 'Exclusive-Or' table of logic, choosing between two options in which the correct answer could be one or the other, but neither nor both.

The solution to this problem is to add at least one *hidden layer* of units between the inputs and the outputs, as shown in Figure 1 below. That architecture, with weighted linear inputs (Eq. 1) followed by a nonlinear transformation (Eq. 2), can produce an arbitrarily complex *nonlinear* mapping between inputs and outputs. Each layer in the network (input, hidden, output) is fully connected to the next one. As will be discussed below, the training methods currently in use are based on error back propagation, which computes the partial derivative of the model output error with respect to each model weight. This requires a *continuous squashing function*, so in place of the *step function* in Eq. 2 it is customary to use the *sigmoid* function of Eq. 3. The sigmoid function is a curve ("S" type) that describes a progression from small beginnings that accelerates and approaches a climax over time. It is call squashing function because they compress an infinite input range into a finite output range.

$$Out_i = \frac{1}{1 + e^{-Netj}} \quad \text{.....Eq. 3}$$

The output activation Out_j of each hidden and output node is calculated using the sigmoid quashing function of Eq. 3 to generate an output as a real value in the range between 0 and 1. The value of the activation Out_j represents the new signal that is to be transferred to the next layer. [12, 13].

The most common way to compute the error between each layer is called error back propagation [14]. Using sum of squares of the arithmetic differences between the output and the target value (*SSQ*) during training, a correction weight is generated to improve the performance of the network. This correction is propagated from the last layer, to the hidden layer and finally to the input layer, using the Chain Rule of calculus to compute the gradient of SSQ_j with respect to each weight in the network. It is also called Gradient Descent. Details can be found in references [12, 13, 14, 15]. Call this update rule the *Delta Rule*, with update weights denoted by ΔW[gd], where all weights are subsumed into W and 'gd' signifies the weight change computed with Gradient Descent.

The conventional implementation of the Delta Rule is given by the *heuristic* in Eq. 4:

$$W^{n+1} = W^n + \eta \Delta W[gd] + \alpha (W^n - W^{n-1}) \quad \text{.....Eq. 4}$$

The change of weights between one iteration and the next, (W^{n+1} - W^n), is η [learning rate] times the Gradient Descent weight change plus α [momentum] times the previous weight change. The learning rate must be adjusted for the specific problem or perhaps during the training for efficiency, and momentum is reported from some simulations to improve the model's performance by note 'getting stuck' in local minimum [14].

A mathematical model with the feed forward back propagation model preloaded was used for the neural network training and analysis, allowing saving time in the equations programming.

3. Experimental

A full factorial design was created in order to collect data for the training of the ANN. The key variables in the design were the titanium dioxide concentration, pigment volume concentration (PVC) and the properties of the titanium dioxide grade. These variables allow the formulator to create a broad range of formulations.

The design variables were as follows:

1) Pigment volume concentration (30%, 50% & 70%)
2) Titanium dioxide concentrations (60g/l, 160 g/l & 250 g/l)
3) Key properties of titanium dioxide: Oil absorption (OA), Particle size distribution (PSD) and Carbon Black Undertone (CBU). A broad range of these properties was selected using 6 different grades of the

pigment, covering most of the variety of grades found in the market.

The properties measured to the final product were as follows:

- Color L*, a* and b*: the measurement of color using CIE Lab is based on the idea that any color could be created using 3 primary colors (green, red & blue). This system defines a color space that is characterized by an a*-axis (goes from green to red), a b*-axis (goes from blue to yellow) and a L*-axis (goes from black to white) [16].

- Spread rate: this property is defined as the yield of a paint to cover the color or color differences of substrates, on which it is applied. Both light absorption and scattering contribute to the hiding [16].

- Tinting strength: this is the ability of the titanium dioxide to increase the lightness of a colored, gray or black medium, using reflectance measurements and the Kubelka-Munk function to calculate the scattering power [16].

4. Simulation

For the training of the neural network, a database was created with the characterization of the titanium dioxide grades, formulation parameters and the properties of the final coating. All the input and output values were normalized between 0.1 to 0.9 by using linear scaling. This normalization is really important to preventing large number overriding smaller ones and maintaining their values between the limits of the activation function. In the particular case of the sigmoid function, this normalization is advantageous to prevent the networks driving the range to the infinity, slowing the learning process [13].

$$X_s = 0.1 + 0.9\frac{(X - X_{\min})}{(X_{\max} - X_{\min})} \quad \text{.....Eq. 5}$$

The experimental data consisted of 216 experiments, of which 75% was used for training and 25% for the test data set.

The performance of the neural network, with the appropriate number of hidden units, is shown during training for each output below. In all the cases, the training error curve shows a decrease in the error. The optimum model ('weight best') was selected when the test error growth was a minimum or unchanging, avoiding over-parameterization.

5. Results

The goal of the neural network model is to predict, with high accuracy, the architectural coatings properties: spread rate, tinting strength, and color L*, a* and b*. Comparison of the predicted vs. measured data is key to defining the reliability of this model. Minitab was used for the statistical analysis.

Paired T tests were used to test the mean difference between paired observations (modeled and observed). A linear regression analysis was performed to confirm the correlation between the calculated vs. measured data. Finally, a global sensitivity analysis, using the Neural Webkit, was performed to identify the relative importance of the inputs for each output.

The results of this statistical analysis are shown in the figures below.

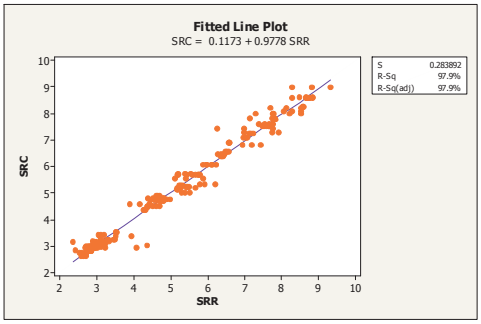

Fig. 1. Linear regression analysis for Spread rate.

The R-Sq for the Spread rate is 97.9%, demonstrating a high correlation for the prediction of this property using this model. The paired T Test showed an insignificant P value, since the means are similar. This is one of the most important properties, because it is directly related to the titanium dioxide type, quality and quantity.

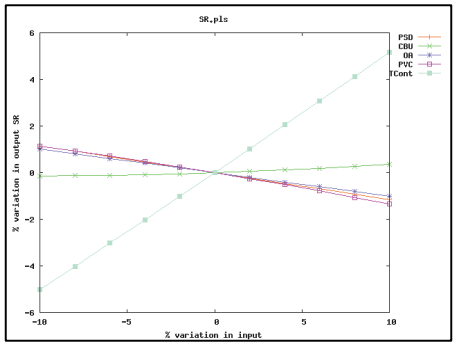

Fig. 2. Global Sensitivity Analysis for SR.

The spread rate of a paint has a very strong correlation with the titanium dioxide content, as this pigment is the main contributor in the total scattering of the visible light in the paint. CBU has a slightly contribution to this output, as the undertone of the pigment could affect apparently the spread rate. Higher CBU could be seen as darker paints. The rest of the inputs have a small negative correlation.

Software was developed using the mathematical model created with the ANN programming in C#. This system allows the formulator or engineer to create virtual formulations of architectural coatings in a graphical environment.

Fig. 3. Initial screen of the system

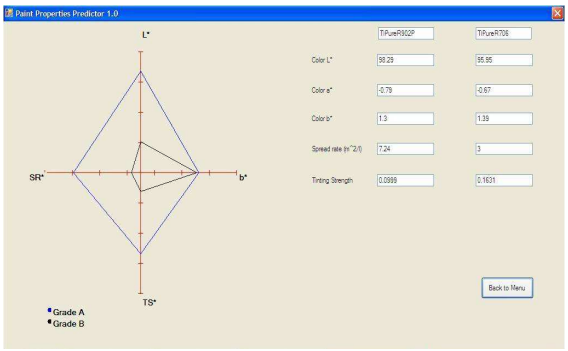

Fig. 4. Properties analysis numerical screen

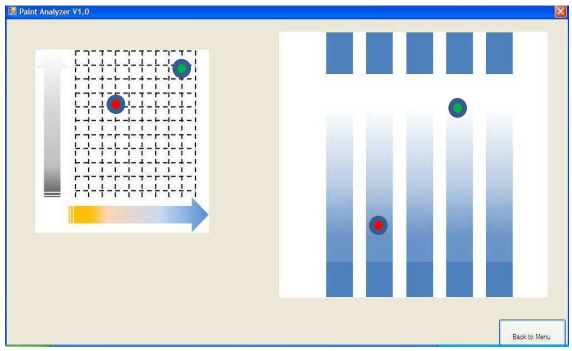

Fig. 5. Properties analysis numerical screen

6. Conclusions

The accuracy of this model for predicting architectural water based coatings properties was demonstrated during training by the RMS error reduction in both the training and test data sets. The statistical analysis performed on the set of calculated vs. measured data confirmed good model predictions. In all of the calculated models for property prediction, the R^2 was larger than 95%.

The characterization of the titanium dioxide grade, as three inputs in the model, proved to be a good approach for predicting the final properties of the architectural coating. Since this is a key element that defines most of the interactions of the visible light with the paint, due to the scattering power of the pigment, this affects the optical properties of the coating.

This model could be generalized to predict the output on unseen test data, as long as the inputs of the model are within the min/max range used.

The scope of future studies is to develop a model which estimates the contribution of the process parameters (impeller & tank diameter, power and tip speed) and the direct effects of other raw materials (resins and fillers) on the final coating's properties, by applying methods similar to those in this report.

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