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EVALUATION OF THE EFFECT OF DRY-FILM BIOCIDES ON PAINT FILM PRESERVATION USING NEURAL NETWORKS

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Abstract - Biocides play an important role in the preservation of a variety of products susceptible to microbiological growth such as paint, a material that can undergo microbial deterioration both in storing (inside the can) and after the application on a surface. In this work, artificial neural networks were used to predict the level of fungal growth on surfaces painted with water-based paints with biocide formulations containing different concentrations of ten kinds of commercial and experimental chemical agents. The use of neural networks is well known in chemical processes and they are a powerful tool for discovering relationships between sets of data. Industrial Environmental Tropical Chamber tests were used as the network training set. The importance of the each additive of the dry-film biocide formulation in prevention of biodeterioration was also examined.
Keywords: Neural networks; Biocide; Paint film; Fungal growth.

INTRODUCTION

Biocides are important in preventing biodeterioration of a variety of products such as cosmetics, pharmaceutical products, polymers and paints. Application of biocides in water-based paints is important because the presence of water, carbon (from resin) and mineral charge (inorganic nutrients) makes this an appropriate place for development of a variety of microorganisms.

Biocides must be added to paint for protection during storing (wet-state or in-can biocides) and surface coating preservation (dry-film or in-film biocides). The largest volume of biocides used falls within these two categories, but there is still another category of biocide used in the paint industry: surface sterilants (Rees, 2001).

During the storage of water-based paints, bacteria that can be present in raw materials such as pigments, fillers and water find an environment that is favorable to their growth. Contamination can also take place due to inadequate asepsis of equipment and storage tanks.

Inside the can, there are places with oxygen (empty space between the paint and can lid) that allow aerobic bacteria and yeast growth and places without oxygen (deep within the paint can) where anaerobic bacteria can grow. The resulting biodeterioration leads to changes in viscosity and pH, production of CO_2 (that can cause foam and swelling of the can) and, if there are sulfate-reducing bacteria, a bad smell resulting from production of H_2S. Microorganisms that can grow in that kind of environment include *Pseudonomas*, *Aerobacter*, *Flavobacterium*, *Escherichia proteus* and *Bacillus sp*. (Kairalla et al., 1993). Addition of chemical biocides for in-can preservation and implementation of a system of good housekeeping can avoid this kind of contamination (Anker and März, 1997).

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After application of paint on a surface, the film may be in contact with fungal spores and algae from the air. This kind of contamination can lead to film spalling and color variation (undesirable aesthetic changes). To avoid this kind of contamination, it is important to use antifungal and antialgal biocides. Inadequate conditions of application of the paint such as surfaces that are dirty, have old coatings or are already contaminated with microorganisms can also contribute towards reducing film durability.

Fungi are particularly dangerous to paint films since, unlike algae, they can develop on both external and internal walls. The literature has pointed to fungi as the major microorganism responsible for microbiological spoilage of painted surfaces (Shirakawa et al., 2002b). Examples of fungi that can grow in paint films are *Aspergillus niger*, *Cladosporium* and *Alternaria* (Kairalla et al., 1993). Shirakawa et al. (2002a) described the natural sequence of fungal colonization on two buildings in the South-east of Brazil, which were painted with an acrylic paint with and without a broad-spectrum biocide formulation, by experimental observation over a 42-week period. The main fungal genus detected by those authors was *Cladosporium* and, for the first time, the genus *Tripospermum* was reported on painted buildings.

Some algae that can develop on painted surfaces are from the *Chlorophyceae* and *Cyanophyceae* families and examples of lichens (symbionts between fungi and algae) are *Bryophytes*, *Pterodophytas* and *Spermatophytes* (Kairalla et al., 1993).

The problem of biocontamination of surfaces has attracted the attention of several researchers in the past several years. Gaylarde and Gaylarde (2000) found algae, cyanobacteria, protozoa, fungi, slime, moulds, actinomycetes and other bacterial groups on surfaces of painted buildings in five Latin American countries (a total of 1363 different morphotypes were found by the authors). These authors suggested that there are approximately 4×10^6 species of phototrophs on painted walls throughout the world. Gutarowska and Zahowska (2002) proposed a mathematical model that describes a correlation between the amount of ergosterol (a basic sterol of cellular membranes in filamentous fungi and yeast) and the number of colony-forming units of mould growing on building materials such as concrete and emulsion coat. Bjurman (1999) employed sensitive methods for determination of microbial colonization of external walls covered with three paint systems. Clarke et al. (1999) formulated a mould growth model based on six generic mould categories in terms of the minimum combination of temperature and relative humidity for which growth will occur on building materials.

Isothiazolinone-based biocides are among the most widely used biocides for paint protection (Rees, 2001; Anker and März, 1997). The initial biological activity of the isothiazolinones is thought to arise from their ability to readily pass into membranes and fungal cell walls and then react with important intracellular sulfur-containing proteins or simpler molecules inside the cell, causing impairment of cell function (Morley et al., 1998).

Shirakawa et al. (2002b) tested six biocides separately incorporated into phosphogypsum (a residue of phosphoric acid produced from apatite that is incorporated into building materials) specimens and found that the biocide 2-n-octyl-4-isothiazolin-3-one was the most efficient compound for those specimens tested. The authors also found that the fungus *Helminthosporium sp*. was the most resistant fungus tested, showing growth on all biocide-containing specimens tested.

For years, industries have strived to reduce waste due to commercial competition, which necessitates a reduction in costs, and also to environmental considerations and stringent laws being implemented in many parts of the world. Thus the preservation of materials and products that can undergo microbial deterioration such as paint films becomes indispensable. Some microorganisms can also be a human health hazard. Some fungi, for example, can be associated with problems such as allergenic diseases, disorders of the skin and respiratory problems (Gutarowska and Zahowska, 2002; Shirakawa et al. 2002a and 2002b). As the biodiversity of painted building surfaces can be very high (Gaylarde and Gaylarde, 2000), it is necessary to develop biocides with a broad range of action and ever greater efficiency, but with less toxic effects.

To reach these goals, biocide producers are investing in the development of new blends of existing active agents, since developing a new compound involves high costs and time (Rees, 2001; Hume and Moore, 1999). Increasing regulation governing the introduction of new chemical entities has also tended to increase reliance on established biocides rather than encouraging the development of novel antimicrobials (Gilbert and Brown, 1995). By combining existing biocides, producers are also striving to enhance antimicrobial action (synergistic behavior). However prediction of how much microbial growth that a certain combination of several biocides will avoid is not an easy task. Thus, the formulation of highly efficient chemical biocides is still a challenge for biocide and paint producers.

In this work, the efficacy of biocide formulations in preventing fungal growth on paint films was evaluated using artificial neural networks. Biocide blends were formulated with ten different kinds of active agents and added to water-based paints. In other words, we propose a new method based on neural networks to predict the level of microbiological growth, knowing the composition of the biocide blend.

Neural Networks

Artificial neural networks are computational tools which have the ability to learn the behavior of a process and the relationship between groups of variables without any phenomenological model of the system. Their use is well known in chemical processes and they are a powerful tool for discovering relationships between sets of data. The artificial neural networks are also referred to as neurocomputers, connectionist networks, parallel distributed processors (Haykin, 1999) and computational neural networks (Sumpter and Noid, 1996; Hajmeer et al., 1997). This artificial intelligence method has attracted considerable attention because it can handle complex, nonlinear problems and requires less processing time than conventional methods. Some authors have declared neural networks to be as one of the greatest computational tools ever developed (Baughman and Liu, 1995).

A neural network derives its computing power through its massively parallel distributed structure and its ability to learn and therefore generalize (Haykin, 1999).

Many works have demonstrated the potential of neural networks to handle microbiological problems. Morgan et al. (1998) explored the ability of neural networks to identify fungi, employing morphometric data from spores of the *Pestalotiopsis* species and some species in the related genera *Truncatella* and *Monochaetia*. These authors showed that neural networks have considerable potential and compare favorably with other approaches. Another study (Tomáz-Vért et al., 2000) demonstrated the possibility of using a simple neural network for discriminating antibacterial activity of compounds according to their structures with a high percentage of correct classifications. Neural networks developed for prediction of anaerobic growth of the bacterium *S. flexneri* on foods (predictive microbiology) have yielded better agreement with experimental data than have data from nonlinear regression equations (Hajmeer et al., 1997).

Neural networks have been used in many systems; however, with respect to the paint field, not much attention has been paid to the utilization of neural networks and few articles on both neural networks and paints could be found. One example is modeling and optimization of a recipe for paint coating (Zupan and Gasteiger, 1993). In that work, the authors successfully applied neural networks to relate conditions and ingredient quantities (concentration of the polymer component, concentration of the catalyst and temperature used for heating the product) with six properties of a paint coating (hardness, elasticity, adhesiveness, resistance to methy-isobutyl-ketone, stroke resistance and contra-stroke resistance).

In this work neural networks were used to study the effect of dry-film biocides on preservation of paint films. Supervised learning was used. This paradigm uses vector pairs (input and output patterns) in its internal processing in order to minimize the difference between network output and desired output (Sumpter and Noid, 1996).

A typical supervised network (multilayer perceptron) is composed of layers (input, hidden and output) with processing elements (neurons) interconnected by weights. A real number is associated with each weight. Polarization or bias (weight of a neuron that has a constant value, usually one) can also be added. Its purpose is to provide a reference value for all the neurons in the same layer (Twu and Lee, 1995). The input signal propagates through the network in a forward direction on a layer-by-layer basis.

Neural network operations consist of a learning or training phase and a test, generalization or validation phase. During the learning phase, the network is repeatedly presented with a set of input-output patterns (training data set). The learning or network training phase basically consists of an adjustment of weights to minimize the error between the network outputs and the measured (target) values. Validation consists of presenting to the network a new set of data not involved in the training phase. Once validated, the network can be used to predict outputs from new inputs.

The procedure used to perform the learning process is called a learning algorithm. Basically, learning algorithms differ from each other in the way in which the adjustment of the weight of a neuron is formulated (Haykin, 1999). One of the most commonly used algorithms for the supervised training of multilayer perceptrons is the backpropagation algorithm, because of its proven history of success and its ease of implementation

(Sumpter and Noid, 1996). The equations that describe this algorithm can be found, for example, in Savkovic-Stevanovic (1994) and Hoskins and Himmelblau (1988).

MATERIALS AND METHODS

Experimental Data

Data were obtained from experiments based on the Environmental Tropical Chamber test (ASTM, 1986) from Ipel - Itibanyl LTD., a biocide producer. Tests for fungal growth consisted of applying a paint film with the selected biocide on properly prepared *Pinus elliote* wood panels. Panels were placed in an adequate environmental chamber with controlled humidity and temperature, and a solution with a high concentration of a pool of microorganisms was sprayed on the panels. Application of the pool of microorganisms was repeated after seven days. The test was finished after 28 days. Tests were carried out in duplicate. The exposed panels were evaluated for fungi growth and the results of these examinations were rated on a scale of 0-5, as shown in Table 1.

Methodology for Network Training, Validation, Prediction and Calculation of the Influence of Active Agent on Microbiological Growth

The artificial neural network output is the level of fungal growth. The ANN was trained with ten neurons in the input layer (concentration of ten biocides). One hidden layer and sigmoidal transfer functions were adopted. The ANN output is trained to fit the scores. The calculation for truncating the ANN output (a real number) is obtained by simple adjustment (by a decimal), from a real number to an integer.

The training pattern file consisted of 32 input-output examples and the test file (Table 2) consisted of ten data (validation). The validation data set is shown in Table 3. Letters from A to J denote the active ingredients. Their chemical structures will not be revealed because that is an industrial secret.

A neural network computer code was used to simulate the process. The simulator was based on the backpropagation algorithm and includes subroutines to randomize the training data set rows, preprocess data (normalization), test learning efficacy, select the optimal network configuration (number of hidden neurons and two network parameters: learning rate and momentum coefficient) and calculate the relative importance of each active agent in control of microbiological growth by the Garson equation shown below.

$$I = \frac{\sum_{i=1}^{Nhid}\left[\left(\left|W_j\right| / \sum_{k=1}^{Ninp} W_{j,k}\right)\times\left|WL_j\right|\right]}{\sum_{i=1}^{Ninp}\left\{\sum_{j=1}^{Nhid}\left[\left(\left|W_{i,j}\right| / \sum_{k=1}^{Ninp}\left|W_{i,j,k}\right|\right)\times\left|WL_j\right|\right]\right\}} \quad (1)$$

In the above equation, I is the relative importance, N_{hid} is the number of neurons in the hidden layer, N_{inp} is the number of neurons in the input layer, $|W_j|$ is the absolute value of the input-hidden weight and $|WL_j|$ is the absolute value of the hidden-output weight.

The initial weights of the network were assigned small random values. After the network training and validation phases were concluded, ten different combinations of the biocides were arbitrarily chosen (Table 4) and the neural network made the microbiological growth predictions (prediction phase). After that, samples of paints formulated with those chosen biocide blends were prepared and tested in the Environmental Tropical Chamber. Experimental results obtained over a 28-day period were compared with network predictions.

Table 1: Rating scheme used in evaluation of the environmental test.

Rating	Microbiological growth (% of growth on specimen area)
0	no growth
1	less then 10
2	10 – 30
3	30 – 50
4	50 – 70
5	more than 70

Table 2: The data used for the ANN training

	Active agent (ppm)										Biological growth	
Blend	A	B	C	D	E	F	G	H	I	J	Experimental	Neural Network
1	315.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	2
2	675.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0
3	135.0	0.0	12.0	8.4	0.0	0.0	0.0	0.0	22.5	1939.0	2.0	2
4	90.0	0.0	0.0	16.8	0.0	0.0	0.0	0.0	0.0	418.0	3.0	3
5	72.0	0.0	0.0	0.0	160.0	95.0	0.0	0.0	0.0	0.0	2.0	2
6	0.0	0.0	140.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	5
7	47.2	0.0	0.0	2.1	0.0	0.0	0.0	0.0	15.0	1292.5	4.0	4
8	45.0	0.0	0.0	8.4	0.0	0.0	0.0	0.0	0.0	209.0	5.0	4
9	84.4	136.5	0.0	17.5	0.0	0.0	0.0	0.0	0.0	350.0	3.0	2
10	36.0	0.0	0.0	0.0	80.0	47.5	0.0	0.0	0.0	0.0	4.0	4
11	0.0	1800.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0
12	0.0	0.0	48.0	5.6	0.0	0.0	0.0	0.0	0.0	368.5	3.0	5
13	402.0	0.0	0.0	44.1	581.8	0.0	207.8	0.0	7.0	819.0	0.0	0
14	60.7	0.0	8.8	4.2	0.0	0.0	0.0	0.0	0.0	225.0	5.0	4
15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	600.0	0.0	0.0	1.0	1
16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	300.0	0.0	0.0	4.0	3
17	78.7	0.0	0.0	3.5	0.0	0.0	0.0	0.0	0.0	500.0	3.0	4
18	87.8	96.0	0.0	14.0	0.0	0.0	0.0	0.0	0.0	280.0	2.0	3
19	135.0	0.0	0.0	10.5	0.0	0.0	0.0	0.0	0.0	1698.1	2.0	2
20	0.0	0.0	0.0	14.0	0.0	0.0	0.0	120.0	0.0	200.0	2.0	3
21	90.0	0.0	0.0	0.0	0.0	0.0	95.0	0.0	0.0	0.0	4.0	4
22	64.8	0.0	0.0	11.2	0.0	0.0	0.0	0.0	1.6	261.1	3.0	3
23	0.0	600.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	3
24	121.5	0.0	18.0	4.2	0.0	0.0	0.0	0.0	22.5	1862.0	3.0	3
25	81.0	0.0	0.0	4.2	0.0	0.0	0.0	0.0	0.0	276.3	4.0	4
26	10.8	0.0	0.0	10.5	23.5	14.2	0.0	0.0	0.0	150.0	4.0	4
27	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	400.0	0.0	5.0	5
28	40.5	0.0	3.0	4.2	0.0	0.0	0.0	0.0	0.0	225.0	4.0	4
29	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	4
30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	200.0	0.0	5.0	5
31	81.0	0.0	12.0	5.6	0.0	0.0	0.0	0.0	0.0	300.0	4.0	4
32	0.0	0.0	280.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	5

Table 3: Validation data set

	Active agent (ppm)										Biological growth	
Blend	A	B	C	D	E	F	G	H	I	J	Experiment	Neural networks
1	94.5	0.0	0.0	4.2	0.0	0.0	0.0	0.0	0.0	276.3	3	4
2	131.8	144.0	0.0	21.0	0.0	0.0	0.0	0.0	0.0	420.0	2	2
3	0.0	0.0	36.0	4.2	0.0	0.0	0.0	0.0	0.0	276.3	4	4
4	135.0	0.0	0.0	0.0	0.0	0.0	142.5	0.0	0.0	0.0	3	4
5	54.0	0.0	24.0	5.6	0.0	0.0	0.0	0.0	0.0	300.0	4	4
6	14.4	0.0	0.0	14.0	32.3	19.0	0.0	0.0	0.0	200.0	3	3
7	92.8	168.1	0.0	14.0	0.0	0.0	0.0	0.0	0.0	350.0	3	3
8	78.7	0.0	0.0	3.5	0.0	0.0	0.0	0.0	18.7	1740.6	3	3
9	108.0	0.0	0.0	5.6	0.0	0.0	0.0	0.0	0.0	368.5	3	3
10	111.3	201.7	0.0	16.8	0.0	0.0	0.0	0.0	0.0	420.0	2	2

Table 4: Prediction data set

	Active agent (ppm)										Fungal growth	
Blend	A	B	C	D	E	F	G	H	I	J	Experiment	Neural networks
1	94.5	0.0	0.0	21.0	0.0	0.0	0.0	0.0	0.0	1200.0	2	2
2	40.5	0.0	18.0	4.2	0.0	0.0	0.0	0.0	0.0	225.0	4	4
3	162.0	0.0	0.0	8.4	0.0	0.0	0.0	0.0	0.0	552.7	2	2
4	135.0	0.0	0.0	25.2	0.0	0.0	0.0	0.0	0.0	627.0	2	2
5	97.2	0.0	0.0	19.2	0.0	0.0	0.0	0.0	2.4	391.6	2	2
6	196.8	0.0	0.0	19.6	551.2	0.0	196.8	0.0	26.2	0.0	1	1
7	0.0	0.0	0.0	10.5	0.0	0.0	0.0	90.0	0.0	150.0	4	4
8	63.0	0.0	0.0	14.0	0.0	0.0	0.0	0.0	0.0	800.0	3	3
9	54.0	0.0	4.0	5.6	0.0	0.0	0.0	0.0	0.0	300.0	3	4
10	126.0	0.0	0.0	5.6	0.0	0.0	0.0	0.0	0.0	368.5	2	3

RESULTS AND DISCUSSION

Initially the network simulator preprocessed the data (randomization of training data rows and normalization of variables). As discussed in Bishop (1994), one of the most important factors in achieving a successful application of a neural network is the use of appropriate data preprocessing and representation. A better network performance was found when, during training, the target values used for the output neurons were set to range from 0.1 to 0.9 rather than the expected 0 to 1 for sigmoidal transfer functions. If the values 0 and 1 are used as target values, the transfer function tends to generate infinitely high weight values, which can produce truncation errors, causing the weights to become frozen (Hoskins and Himmelblau, 1988). After finishing the training, the outputs of the network must to be post-processed in a similar way to convert them to physically meaningful quantities.

After those operations, training and validation errors were simultaneously obtained for a high number of epochs (computational iterations), which made it possible to observe the evolution of errors. Some randomizations of rows were made during the training phase. The training was finished when the average independent validation error starts to rise (stopping criteria), indicating the onset of overfitting (Swingler, 1996). Overfitting the data means that the peculiarities of the training set are accurately modeled and the network will not achieve a good generalization for new data (Anderson, 1995).

The simulator identified the smallest validation error and, using neural weights corresponding to that epoch, made predictions for the validation data set. Results were then compared to target values.

All these steps were repeated for several values of hidden neurons, learning-rate parameter and momentum coefficient (neural network parameters). Learning-rate parameter is a gain term and momentum is a parameter that smoothes the effect of dramatic weight changes (Hoskins and Himmelblau, 1988).

Table 3 shows a comparison of the predicted and experimental fungal growth for the ten blends of the validation set. The rating scheme used to evaluate the environmental test is shown in Table 1.

As can be seen in Table 3, there is a high percentage of correct classifications (80%). Although it has been pointed out in the literature that the growth of microbes in laboratory media can produce organisms that differ widely from those *in situ* (Gilbert and Brown, 1995), the Environmental Tropical Chamber test is widely used by both paint manufacturers and paint biocide manufacturers. For this reason, results from this kind of test were chosen as the data set for the neural network. However, results of the Tropical Chamber test do not show a very high confidence level and, when tests are carried out in duplicate or triplicate, results that deviate by one unit (for example, duplicate tests can show results 2 and 3 for the same paint) can be found. This is in agreement with the adopted standard, which obeys the following criteria: (i) repeatability: two estimations, each one the central value of a test, obtained for the same operator, may be considered suspect if they deviate by more than one unit and (ii) reproducibility: two estimations, each one the central value of a test, obtained in different laboratories may be considered suspect if they deviate by more than two. This has been accepted for years by both paint biocide manufacturers and their customers. When a neural network has been trained with a data set that contains errors, it is accepted that, when presented with new data, the network will not match them completely. On the other hand, the network results are within the range of experimental error since, for the ten available blends, the two incorrect results (blends 1 and 4) deviate from the Tropical Chamber results only by one. It is interesting to observe that, for evaluation of biocide efficacy using a Tropical Chamber test, it is necessary that an experienced analyst make use of special equipment and properly prepare the paint samples. Tropical Chamber tests take 28 days. Neural networks performed all predictions in a few minutes and required only a conventional computer. The only physical expertise needed to prepare an artificial neural network is to define the important inputs and outputs of the system (Elgibaly and Elkamel, 1998). For these reasons, a percentage of 80% correct classifications for the validation data set can be considered very good, indicating that the neural network is able to make confident predictions for new blends.

Figure 1 shows a weight histogram, in which one can see a weight distribution (a majority of low weights) that is in agreement with what would be expected for a well-trained network (Swingler, 1996). According to Swingler (1996) a healthy weights histogram will show a hump around the values with low magnitude (those near zero) indicating that most of the weights are low. In the opposite way, a histogram with peaks at the extremes of the horizontal axis has probably overfitted the data.

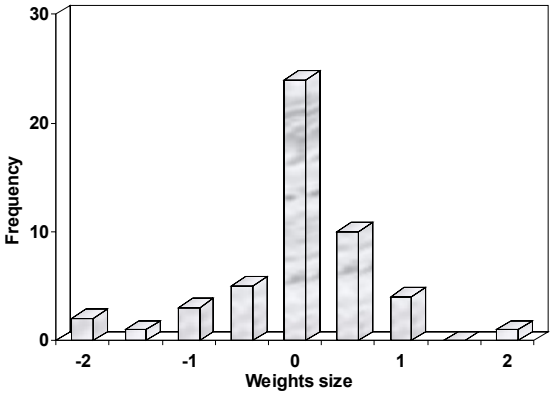

Figure 1: Weights histogram.

Although connection weight does not have any physical meaning, as it is a variable from a black box model, using connection weights it is possible to evaluate the influence of each active agent in the biocide for control of the biological contamination on paint films. Calculations were made by the method described in Garson (1991). Although it is a simple method, it shows that, besides the ability to make predictions, using neural networks it is possible to extract information on how inputs are related to outputs by means of connection weights. It is interesting to observe that bias connections are not included in the procedure. Results are shown in Table 5 and reveal that the primary factor influencing the level of microbiological growth is agent A (18%), followed by agent B (17%). Substances G and J seem to be the least important ones.

Table 5: Influence of active agents (network inputs) for control of microbiological growth

Active agent	Relative importance (%)
A	18
B	17
C	13
D	8
E	8
F	6
G	5
H	12
I	7
J	5

Results in Table 5 are important because they can help the formulator to develop optimized biocide blends. Knowing the factors affecting the control of the contamination, one can use smaller amounts of the active agents and produce a safer product. This is extremely important since, although biocide is fundamental for paint protection, there are warnings in the literature that the use of some biocides can lead to undesirable consequences such as toxic effects (Jayjock et al., 1996) and a prevalence of antibiotic-resistant microorganisms (Fraise, 2002).

Table 4 shows biocide concentrations of the chosen blends in the prediction phase. After neural network simulations, biocide blends were formulated in the laboratory following these concentrations. Several paint samples were prepared and only those which showed stability and could be used under real conditions were selected. Paints were evaluated in the challenge test. Results from experiments and computational simulations are compared in Table 4. As can be seen, 80% of the network predictions match the experimental results. For the selected blends, the incorrect network results (products 9 and 10) differ from the expected results by one unit. As previously discussed, the results obtained are acceptable considering also that biological contamination can be influenced by several factors, many of which are related to sample manufacturing. Of these, changes in the pH of the paints, previous microbiological contamination, effects of redox chemistry (Gillatt, 2000) and lixiviation conditions can be mentioned.

CONCLUSIONS

Water-based paints are very susceptible to microbial deterioration. In this study, we successfully developed a neural network model to predict microbiological growth on water-based paints as a function of the chemical compositions of ten biocides. The results presented in this paper indicate that the neural network is a valuable tool for prediction of microbial growth on paints, being both dependable and fast. The proposed technique is also practical and cost-effective.

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REFERENCES

American Society of Testing Materials - ASTM, Standard test method for resistance of mould on the surface of interior coatings in an environmental chamber. ASTM-D-3273 (1986).

Anderson, J. A., An Introduction to Neural Networks. MIT Press. USA (1995).

Anker, W. and März, R., Desinfection and Preservation in Production of Water-based Paints. Proceedings of 5th International Paint Congress. São Paulo (1997).

Baughman, D. R. and Liu, Y. A., Neural Networks in Bioprocessing and Chemical Engineering. Academic Press. USA (1995).

Bishop, C. M., Neural Networks and their Applications. Review of Scientific Instruments, N° 65, 1803 (1994).

Bjurman, J., Fungal and Microbial Activity in External Wooden Panels as determined by Finish, Exposure, and Construction Techniques. International Biodeterioration & Biodegredation, 43, 1 (1999).

Clarke, J. A., Johnstone, C. M., Kelly, N. J., McLean, M. C., Anderson, J. A., Rowan, N. J. and Smith, J. E., A Technique for the Prediction of the Conditions leading to Mould Growth in Buildings. Building and Environment, N° 34, 515 (1999).

Elgibaly, A. A., Elkamel, A. M., A New Correlation for Predicting Hydrate Formation Conditions for Various Gas Mixtures and Inhibitors. Fluid Phase Equilibria, N° 152, 23 (1998).

Fraise, A. P., Biocide Abuse and Antimicrobial Resistance - a Cause for Concern? Journal of Antimicrobial Chemotherapy, N° 49, 11 (2002).

Garson, G. D., Interpreting Neural-Networks Connection Weights. AI Expert, 47 (1991).

Gaylarde, P. M. and Gaylarde, C. C., Algae and Cyanobacteria on Painted Buildings in Latin America. International Biodeterioration & Biodegredation, N° 46, 93 (2000).

Gilbert, P. and Brown, M. R. W., Some Perspectives on Preservation and Desinfection in the Present Day. International Biodeterioration & Biodegredation, N° 36, 219 (1995).

Gillatt, J., The Effect of Redox Chemistry on the Efficacy of Biocides in Polymer Emulsions. Tintas e Vernizes, 46 (2000).

Gutarowska, B. and Zakowska, Z., Elaboration and Application of Mathematical Model for Estimation of Mould Contamination of some Building Materials based on Ergosterol Content Determination. International Biodeterioration & Biodegredation, N° 49, 299 (2002).

Hajmeer, M. N., Basheer, I. A. and Najjar, Y. M., Computational Neural Networks for Predictive Microbiology II. Application to Microbial Growth. International Journal of Food Microbiology, N° 34, 51 (1997).

Haykin, S., Neural Networks, A Comprehensive Foundation. 2nd edition. Prentice Hall. USA (1999).

Hoskins, J. C., and Himmelblau, D. M., Artificial Neural Network Models of Knowledge Representation in Chemical Engineering. Computers & Chemical Engineering, N° 12, 881 (1988).

Hume, C. and Moore, S. K., Specialties: Biocides - European Directive will Push up Costs. Chemical Week, N° 161, 46 (1999).

Jayjock, M. A., Hazelton, G. A., Lewis, P. G., and Wooder, M. F., Formulation Effect on the Dermal Bioavailability of Isothiazolone Biocide. Food and Chemical Toxicology, N° 34, 277 (1996).

Kairalla, R. B., Ferracioli, A. C. and Alfinito Filho, C., Additives for Preservation, Paint and Varnish. Science and Technology, N° 1, 568 (1993).

Morgan, A., Boddy, L., Mordue, E. M. and Morris, C. W., Evaluation of Artificial Neural Networks for Fungal Identification, Employing Morphometric Data from Spores of *Pestalotiopsis* species. Mycological Research, N° 102, 975 (1998).

Morley, J. O., Oliver, A. J. and Charlton, M. H., Theoretical Studies on the Biocidal Activity of 5-chloro-3-isothiazolone, Journal of Molecular Structure, N° 429, 103 (1998).

Rees, R., New Generation Isothiazolone Biocides: a Result of Responsible Vision for the Future Advancement of the Biocide & Surface-Coatings Industries. Proceedings of 7th International Paint Congress. São Paulo (2001).

Savkovic-Stevanovic, J., Neural Networks for Process Analysis and Optimization: Modeling and Applications. Computers & Chemical Engineering, N° 18, 1149 (1994).

Shirakawa, M. A., Gaylarde, C. C., Gaylarde, P. M., John, V. and Gambale, W., Fungal Colonization and Succession on Newly Painted Buildings and the Effect of Biocide. FEMS Microbiology Ecology, N° 39, 165 (2002a).

Shirakawa, M. A., Selmo, S. M., Cincotto, M. A, Gaylarde, C. C., Brazolin, S. and Gambale, W., Susceptibility of Phosphogypsum to Fungal Growth and the Effect of various Biocides. International Biodeterioration & Biodegredation, N° 49, 293 (2002b).

Sumpter, B. G. and Noid, D. W., On the Design, Analysis, and Characterization of Materials using Computational Neural Networks. Annual Review Materials Science, N° 26, 223 (1996).

Swingler, K., Applying Neural Networks: A Practical Guide. Academic Press. London (1996).

Tomás-Vert, F., Pérez-Giménez, F., Salabert-Salvador, M. T., García-March, F. J. and Jaén-Oltra, J., Artificial Neural Network Applied to the Discrimination of Antibacterial Activity by Topological Methods. Journal of Molecular Structure, N° 504, 249 (2000).

Twu, J. T. and Lee, L. J., Application of Artificial Neural Networks for the Optimal Design of Sheet Molding Compound (SMC) Compression Molding. Polymer Composites, N° 16, 400 (1995).

Zupan, J. and Gasteiger, J., Neural Networks for Chemists. VCH Publishers. Germany (1993).