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Prediction and optimization of fireproofing properties of intumescent flame retardant coatings using artificial intelligence techniques

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ABSTRACT

A multi-structured architecture of artificial intelligence techniques including artificial neural network (ANN), adaptive neuro-fuzzy-inference-system (ANFIS) and genetic algorithm (GA) were developed to predict and optimize the fireproofing properties of a model intumescent flame retardant coating including ammonium polyphosphate, pentaerythritol, melamine, thermoplastic acrylic resin and liquid hydrocarbon resin. By implementing ANN on heat insulation results of coating samples, prepared based on a L_{16} orthogonal array, mean fireproofing time (MFPT) values were properly predicted. The predicted data were then proved to be valid through performing closeness examinations on fuzzy inference systems results regarding their experimental counterparts. However, the possible deviations tapped into phenomena like foam detachment and char cracking were alleviated by ANFIS modeling embedded with pertinent fuzzy rules based on the sole and associative practical role of used additives. The contribution of each intumescent coating component on the formulation with optimized fireproofing behavior was then explored using GA modeling. A similar optimization procedure was also conducted using conventional Taguchi experimental design but the GA based optimized intumescent coating was found to exhibit higher MFPT value than that suggested by the Taguchi method.

1. Introduction

The ever-increasing demand for advanced fire-protection systems in finish industry has significantly altered the performance profile required of modern flame retardants and led coating formulators to focus on developing novel classes of products. Intumescent coatings, as a result, represent a technical, environmentally sound and economical way to offer flame protection, together with a striking architectural appearance [1–4]. Intumescent flame retardant formulations are normally constituted of three main components comprising an acid donor, a carbon donor and a blowing agent, bounding with each other by a polymer binder [1–4]. In a real fire situation, in the first step, the macromolecular binder melts to facilitate the foam expansion process [5]. Subsequently, the acid donor component decomposes to a mineral acid, providing the basis for the formation of carbonaceous char [5]. Once the blowing additive breaks down and volatilizes, this char layer expands and gradually forms a swollen cover on the top of the remaining materials [5]. Such an intumescent layer could play a role as an insulation barrier, protecting the substrate from the heat exposure by fire.

Despite the introduction of various mixtures to develop novel intumescence systems, they mostly fail to meet the practical requirements of standard flame retardants. In this concern, a great deal of efforts has been directed so far to identify the underlying causes for these intumescent coatings to be incompetent [6–8]. The general conclusion emerging from these studies is that a desirable intumescence phenomenon cannot be achieved unless the concentrations of the intumescent additives used in the formulation be chosen properly. For instance, Antia et al. [8] reported that the chemical structure of the final product obtained from the reaction between ammonium polyphosphate (APP), as an acid donor, and pentaerythritol (PER), as a carbon donor, depended on the proportion of PER and APP contents. A PER:APP molar mass ratio of 6:1 resulted in the highest carbon concentration in the charring layer, leading to the maximum efficiency of the intumescent coating.

Nevertheless, even with the valuable guidelines as mentioned above, no practical procedure have so far been introduced to predict and optimize intumescent flame retardants properties. In order to provide a complete and accurate design approach for

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such materials, one may require a large amount of material consumption, high apparatus cost and processing time. Given the aforementioned difficulties, we believed that the introduction and design of a predictive method, being able to deal with complicated relationship and non-linear set of data by employing a small experimental dataset, could provide an important contribution to alleviate this problem.

From the above facts, artificial intelligence (AI) techniques that currently known as powerful tools to deal with polymeric phenomena, seem to fully match the imposed requirements. Foremost among these methods is the artificial neural network (ANN), which tries to explore empirical interactions between the data points [9–11]. One merit of ANNs is their independence from problem-solving algorithms and prior information regarding pertinent chemical and physical rules [12,13]. In addition, due to their robustness, high computational rate and capability to learn patterns, makes ANNs suitable to be administered to model complicated systems [14–16]. From a similar point of view, combined neuro-fuzzy methods are fuzzy-based models using ANNs to embed fuzzy rules and sets through processing input information. A particular advance in neuro fuzzy theory is the adaptive-neuro-fuzzy-inference-system (ANFIS) as a premier integrated neuro fuzzy hybrid model [17,18]. Reaching faster to convergence in comparison with other neuro fuzzy based methods, ANFIS has won great honors in modeling nonlinear data.

From another standpoint, the genetic algorithm (GA) is among the most promising techniques for optimization of non-linear problems, which takes advantages of Darwin's natural selection approach to obtain the optimum formulation. GAs, are computer programs that 'evolve' in ways that resemble natural selection in organisms and solve very complex problems.

The present study reports on the prediction and optimization of fireproofing properties of an intumescent flame retardant coating containing APP, PER, melamine (MEL) as blowing agent, a thermoplastic acrylic resin (TAR) as a binder, a liquid hydrocarbon resin (LHR) as plasticizer and titanium dioxide (TiO_2) as pigment. For experimental plan, a Taguchi orthogonal array was chosen, and the heat insulation tests were then performed on the purposed formulations. Thereafter, a multi-structured ANN and ANFIS architecture as well as a GA method were implemented on the resultant data in terms of mean fireproofing time (MFPT) and foam expansion percentage to carry out the prediction and optimization processes, respectively. A similar procedure was also conducted using conventional Taguchi experimental design, and its results were compared with the GA method.

2. Experimental

2.1. Materials

APP (Exolit AP 422), with a phosphorus content of 31–32% (w/w) and a nitrogen content of 14–15% (w/w) was purchased from Clariant GmbH, Sulzbach, Germany. PER (Penta tech) with a molecular weight of 142.5 g/mol and an OH-value of 1.615 mg KOH/g was supplied by Perstorp Co. Bruchhausen, Germany. MEL with a molecular weight of 126.12 g/mol was obtained from BASF-AG, Ludwigshafen, Germany. Acrylic resin (Tacryl MC25) with a solid content of $58 \pm 1\%$ and a viscosity at 25 °C of 10,000–15,000 cP was supplied by Taak resin Co., Tehran, Iran. TiO_2 powder (KRONOS 2300) with a density of 4100 kg/m^2, a brightness L^* of 97.4 and a tone B^* of 1.5 was purchased from Kronos International Inc., Leverkusen, Germany. LHR (NOVARES LA 700) with density of 1010–1050 kg/m^2 and OH content of 2.3–2.8% was purchased from Rutgers GmbH, Duisburg, Germany. In addition, the substrates used in this study were steel 304 grade panels having dimensions: 3 mm × 70 mm × 150 mm. All the test substrates were degreased with pure acetone and polished with 180 grit sandpaper prior to the coating application.

2.2. Taguchi experimental design

The Taguchi approach can be used as a traditional analysis tool to minimize the number of experiments while retaining quality of data collection. In addition, the analysis of variance on the collected data from the Taguchi experimental design can be used to optimize the performance characteristics. According to the objectives of the present study, five factors were introduced as affecting the flame retardant behavior of the intumescent coatings; these were the APP, PER, MEL, TAR and LHR loadings. Each of these factors was considered to be varying at several levels that are summarized in Table 1. Consequently, from the number of factors and levels that have been selected, an orthogonal array of L_{16} type was used as shown in Table 2.

2.3. Sample preparation

At the beginning, TAR and LHR were mixed through vigorous agitation at room temperature. At the same time, APP, PER, MEL and TiO_2 were mixed and ground for about 1 h in a ball mill to reach a particle size under 10 μm. The resultant compounds, with the formulations presented in Table 2, were mixed together by a high-speed disperse mixer for 3 h. It should be noted that the TiO_2 weight was constant (5 g) in all the compounds. Since the prepared intumescent coatings had a high solid concentration, an airless spray method was used to apply the coating on the steel substrates. For each of the samples, three layers of coatings were applied including an epoxy primer (60 μm thick), an intumescent coating (1000 μm thick) and a top coat (60 μm thick) to protect fire retardant as well as desired color shade. The coated panels were then exposed to fresh air to dry for at least 1 week.

Table 1
Selected factors and their respective levels.

Factor	Level 1 (g)	Level 2 (g)	Level 3 (g)	Level 4 (g)
TAR content	10	11.5	13	14
LHR content	1.5	2.5	3.5	4.5
APP content	21	23	25	27
MEL content	9	10	11	12
PER content	10	11	12	14

Table 2
The L_{16} orthogonal array for selected factors and levels and the corresponding foam expansion percentage for each trial.

Trial no.	TAR (g)	LHR (g)	APP (g)	MEL (g)	PER (g)	Foam expansion (%)
1	10	1.5	21	9	10	1100
2	10	2.5	23	10	11	4100
3	10	3.5	25	11	12	2200
4	10	4.5	27	12	14	1700
5	11.5	1.5	23	11	14	3700
6	11.5	2.5	21	12	12	1700
7	11.5	3.5	27	9	11	2900
8	11.5	4.5	25	10	10	2500
9	13	1.5	25	12	11	3900
10	13	2.5	27	11	10	5000
11	13	3.5	21	10	14	4000
12	13	4.5	23	9	12	3200
13	14	1.5	27	10	12	3500
14	14	2.5	25	9	14	1900
15	14	3.5	23	12	10	1200
16	14	4.5	21	11	11	2100