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HIGH QUALITY EMULSIFIED PAINTS FORMULATION BY MEAN OF A SOFTWARE FOR THE STATISTICAL DESIGN OF EXPERIMENTS

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Summary. The purpose of this work was to evaluate the partial substitution of TiO_2 by any of two synthetic pigments known as vesicular pearls (Beads®,) and opaque polymers (Ropaque®), maintaining the properties and quality of the original paints, by mean of a statistically designed set of experiments using the software Design Expert®. The software was developed using a linear programming model that require the definition of those variables useful for the selection of different alternatives, of the objective function to be optimized, and the restrictions to be applied to guarantee the products quality. The defined response variables were those properties with the highest sensitivity to the amount of TiO_2 used in the paint formula, that is: cracking, white index, contrast ratio, and the cost reduction. The latest was also taken as the minimization objective function. The inlet variables were selected between those with the highest expected influence over the response variables, that is: the main pigment, the three extender pigments, the substitutive technology selected (vesicular pearls or opaque polymers), and the latex resin type. Once the optimal formulations were obtained it was possible to assert that the selected response variables were those that characterize an emulsified paint of the highest quality. The selected inlet variables showed to have a clear and direct influence on the variables that characteristics this paints. The partial substitution of TiO_2 by any of the two substitutive technologies (Beads® y Ropaque®) reached the Standard quality required by the norms that characterize emulsified paints of first quality and at a minor cost.

1 INTRODUCTION

The TiO_2 is the basic pigment used for white paints or for those paints where the white color is an essential part in the mixture for the desired color(Ropaque®)[3]. Due to the increasing TiO_2 costs, the painting industry is suggesting the partial substitution of that oxide by cheaper synthetic pigments like the vesicular pearls (Beads®) and the opaque polymers[2].

The vesicular pearls developed by *Dulux Australia Limited* and patented by *Sherwin-Williams* in 1980[1], are hard spherical polyester particles cross-linked with styrene, with air trapped inside, and covered by a layer of TiO_2 in order to get the maximum opacity. Ropaque®, instead, is an emulsion of acrylic-styrene polymer in the form of spherical opaque pearls filled with water. During the drying process of water based paint with Ropaque ® after being applied to a surface, the water diffuse out of the pearls being substituted by air. The air trapped inside the pearls act for both synthetic pigments as the light dispersion media. This phenomenon caused by differences between the polymer refraction index and that of the air[2,5], enhance the paints covering power.

The emulsified paints components are the *filling pigments* (clay, $CaCO_3$, talc, silica, mica), the *primary pigments* (basically TiO_2), *latex resins* (vinyl-acrylic [Latex 1], styrene–acrylic [Latex 2], and *additives* (coalescent compounds, surfactants, humectants, foaming agents, dispersers, thickening species). Each component is essential in order to obtain the properties that characterize the paints quality[4].

The main objective of this work was to demonstrate how useful is the use of some commercial software like the Design Expert® version 5.0, in order to minimize the amount of new formulations that need to be tested in order to obtain an emulsified first class paint formula were the TiO_2 was partially substituted by the above mentioned synthetic pigments known as vesicular pearls (Beads®) and opaque polymers (Ropaque®), but maintaining the properties and the quality of the original ones.

2 DEVELOPMENT OF A MODEL

Design Expert®, version 5.0, is commercial software that allows the development of statically founded experimental programs. First, a mathematical model must be defined that guarantee the generation of the family of possible formulations for paints with the same performance of the actual paint but at a lower price. The model was developed using linear programming tools, and require the definition of those variables that will allow making a selection, of an objective function to be minimized, and the restrictions that formulations must obey in order to guarantee the product quality. In order to asses how the partial substitution of TiO_2 affects the quality of the paint, it is necessary to make preliminary laboratory experiments based on the standard formulation supplied by the manufacturer.

The objective function to minimize was the cost of production for the emulsified first quality paints, where the TiO_2 is partially substituted by the synthetic pigments Beads® and Ropaque®, maximizing at the same time their quality. The model requires entrance variables to be specified, and it will generate values for response variables. The inlet variables are the paint formulation compounds that have the highest influence on the quality, and the response variables are the product properties that define its quality.

In our case the inlet variables were: the primary pigment (TiO_2), the synthetic pigments (vesicular pearls Beads® or opaque polymer Ropaque®), the three filling pigments (clay, $CaCO_3$ and talc) and the kind of latex resin (vinyl-acrylic or styrene-acrylic) to be used. The response variables were: cracking, white index and contrast ratio. Additionally the software requires the inclusion of the objective function selected, what in our case was the cost of production.

The restrictions for the model were defined trough the volumetric pigment concentration or PVC, which measure the ratio of the pigment volume to the total volume of solids in the paint (pigments plus the other solids in the latex). The PVC value is fixed by the manufacturer in order to fulfill requirements established by regulations, which in our case are “Normas para Fabricación de Pintura de la Comisión Venezolana de Normas Industriales – COVENIN”.

The degree of TiO_2 substitution was determined using the protocol supplied by the supplier of the synthetic pigments. With this information the range TiO_2 substitution was found to lay between 20 and 35%. The range of filler pigments to be used was fixed following the formulation scheme used with the TiO_2. The amount of clay in the formulation should vary from 0 to 50% of the total volume of filler pigments, the remaining being distributed between the $CaCO_3$ and talk in a ratio of 4:1.

The model, inserted into the software, will generate a set of mixtures formulations that will meet the required quality, complying with the objectives and restrictions of the model. The software meet its objective evaluating the mixture formulation set analyzing the variance (by ANOVA), the normal distribution, t-test, the desirability function, the prediction level, the presence of autocorrelations, and the consistency in the error propagation for each involved variable. This procedure will allow identifying those mixture designs that better comply with the specified quality requirement set by the model. Twenty five possible formulations complaining with the model quality specification were obtained and then tested in the laboratory. The software gave the maximum and minimum for each of the model response variables, and with this information the convenience of completing the experiment is assessed. The predicted range should fall within the range for each dependent variable. As a result, a set of optimized formulation were obtained, and from them the one with the lowest cost and the best performance was choused.

The design procedure was executed twice substituting partially the TiO_2 by vesicular pearls (Beads®) in first place and again using opaque polymers (Ropaque®).

3. RESULTS AND DISCUSSION

The results analysis was done considering the four response variables of the model (cracking, white index, contrast ratio, and costs reduction). In all studied cases the cracking behavior was excellent making unnecessary its discussion.

Figure 1 shows results for the new formulations as a percentage of the value obtained with the original formulation. Formulation with Latex 1 leads to lower costs, what is direct consequence of the row material costs. For all cases the lower costs are obtained using Ropaque ®. The contrast ratio show almost the same variation for both latex formulation (differences are lower than 1%), what can be explained because this ratio depends on the TiO_2 to the fillers ratio in the mixture. These values are higher than the values fixed for first quality paints by the COVENIN norms (R.C. = 98%). The value obtained using Ropaque ® is higher than the obtained with Beads ®, what is the consequence of the higher porosity of the dry layer of the paint obtained with the first pigment due to its smaller sizes and a more uniform distribution. The white index response for both latex formulations are also similar, what can be explained because the index is mainly related to the amount of TiO_2 and not to the latex type. It can also be seen that the white index have a tendency to be higher with Ropaque ®, what can be explained because this synthetic pigment is a very white styrene-acrylic emulsion meanwhile the vesicular pearls is a polyester-styrene emulsion with a color tendency toward yellow. It is interesting to point out that Latex 2 do not certify better values for the white index or the contrast ratio than those obtained with the less expensive Latex 1.

It must be emphasized that the quality limits set by the norms are reached with both synthetic pigments with values falling within the range set by the software.

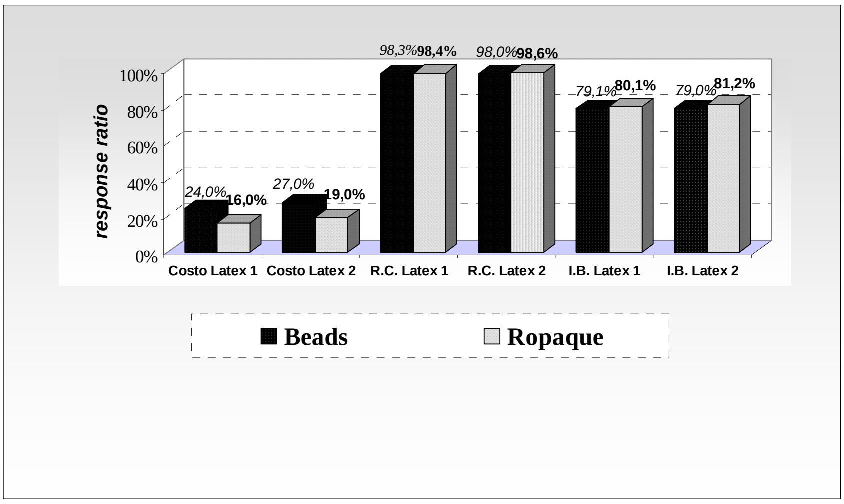

Figure 1: Optimum formulation for both synthetic pigments.

4. CONCLUSIONS

The selected inlet variables (TiO_2, Beads ® or Ropaque ®, clay, $CaCO_3$, talc and vinyl-acrylic or styrene-acrylic) showed a direct impact over the response variables: cracking, white index and the contrast ratio. The partial substitution of TiO_2 in first quality emulsified paints by vesicular pearls (Beads®) or by opaque polymers (Ropaque ®), reached the quality limits required by the norms that rules the emulsified pains manufacture and with a lower production cost. For the same paint quality, the cost reduction is lower with the use of styrene-acrylic (Latex 2) than with the use of vinyl-acrylic (Latex 1). The highest costs reduction is obtained with formulations using opaque polymers (Ropaque ®) and the latex styrene-acrylic.

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