Estimating the modelling of polymer materials’ optical density rate

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Abstract. Mathematical representation of reality is one of the variants of a model as a system, the study of which allows obtaining information about some other system. The mathematical model, in particular, is designed to predict the behavior of a real object. All natural and social sciences that use the mathematical apparatus, in fact, are engaged in mathematical modeling: they replace the object of study with its mathematical model and then study the latter. With the help of mathematical methods, as a rule, an ideal object or process is described, built at the stage of meaningful modeling. The connection of a mathematical model with reality is carried out with the help of a chain of empirical laws, hypotheses, idealizations and simplifications. A mathematical regression model has been developed that takes into account the influence of the speed of printing equipment and pressure on the optical density of the print when printing on non-absorbent surfaces using the gravure printing method.

1 Introduction

Today, the appearance of any product is to some extent associated with packaging products. This is one of the main channels of communication between the manufacturer and consumer of packaging products [1]. Certain standards have been developed for those related to packaging products and product design. Print speed is one of the most important factors affecting the quality of printed products. As the printing speed increases, the contact time of the printed material with the printing plate naturally decreases, which, as can be expected, will lead to a decrease in the amount of ink transferred to the printed material, a decrease in the optical density of the print, i.e. decrease in the quality of printed products [2, 3].

The packaging industry remains the only industry in the world market where production growth has been observed (3.3-3.5% per year) [4]. By 2020, the share of packaging products in the total printing market ($468 billion) has amounted to $157 billion, including packaging boxes, soft packaging. The production of packaging products is expected to grow by 2.6% for flexo printing, and for digital printing by 8% [5].

The share of gravure printing equipment in the world market is 54% in the USA and 45% in Europe. In Turkey, this figure is 70%, and on flexographic printing equipment - 30%. Among the total number of printing equipment in Asian countries, the leading position is occupied by equipment for intaglio printing, i.e. 95%. The reason for this is the possibility of obtaining complex hieroglyphic inscriptions of Asian countries in flexo printing. But in
recent years there has been a significant change in the number of flexographic printing equipment, which is 25% [6].

The current state of development of technology and technology of printing production allows processing and printing on polymer films with different chemical structures. Polymeric materials do not absorb ink, causing a number of wetting and ink adhesion problems [7]. Since almost all polymer films are printed using gravure printing, it is necessary to reconsider all problems associated with printing specifically.

One of the conditions for high-quality printing on the surface of a polymer material is the adhesion of ink to the surface of the material [8]. During processing, the wetting of the film surface is improved, and thus cross-links are formed on the surface with solvents, adhesives, paints, varnishes and extrusion layers. The interaction of paint and polymeric material depends on several parameters.

The ink must wet the surface of the resin film in order for the printed material to form a durable layer [9]. Printing ink is evenly applied to the surface of the material. As a result of the evaporation of organic solutions, the paint transferred to non-absorbent surfaces is fixed. The nature of the print is the interaction of ink with the printed material, that is, the amount of transition of a certain part of the ink layer to the printed material. The quantitative characteristic of the ink is the critical thickness of the ink layer on the printed material, corresponding to the optimal value of the optical density of prints [10].

It is difficult to use only optical density to control the quality of a printed print, it depends on the ink layer, and the ink layer itself is directly related to the surface of the printed material. In the production process of printed products, the assessment of ink transfer in copies is carried out in a subjective form, which increases the time spent on identifying defective prints [7]. Therefore, the development of a model for transferring ink to multilayer polymeric materials by gravure printing is of great scientific interest.

Ensuring accurate color reproduction in gravure prints is one of the main parts of the problem. One way to solve this problem is to create effective color management tools that are an integral part of the printing industry, which increases the productivity of printing equipment, reduces the cost of prepress processes, and reduces the amount of rejected prints, which increases the overall productivity of the print production [4].

Quality control scales are an integral part of the printing process. In such scales, all densitometric parameters of the elements (solids, individual color areas of the raster and their combination, areas for measuring ink transfer, growth of raster dots during printing, color control areas, image blur, etc.) are included as the basis for the final assessment of product quality and its control in the production process [6].

Rigid packaging is a rapidly growing adaptable packaging industry. This is due to the desire of consumers to use convenient packaging, distinguished by the ease of production of vertical hard bottom packages and the ease of opening. Due to their lightness, vertical packaging, on the one hand, saves raw materials, and on the other hand, reduces transport costs. In addition, modern packaging technologies with the help of packages with a sterilized bag provide an improvement in the quality of products and the speed of their filling [2].

As the speed of printing increases, a number of factors affect the transfer of ink from the printing plate to the printed material. Decreasing contact time with increasing print speed can reduce ink transfer to the printed material, which in turn can reduce optical density. At the same time, the increase in pressure caused by the increase in print speed reduces the amount of ink passing through the printed material [9].

The displacement of the maximum area at the beginning of the contact path contributes to the reduction of the inkability of the printed material (the unevenness and porosity of the printed material collapses much earlier, because the printing ink is suddenly in a high pressure zone in the contact path). Printing ink does not have time to penetrate into the pores and irregularities, but remains on its surface.
2 Materials and methods

To develop a mathematical regression model that takes into account the effect of the speed and pressure of printing equipment on the optical density of printed impressions when printing on the surfaces of polymeric materials using the gravure printing method, laminated multilayer composite materials were selected:

1. BOPP/OPP (biaxially oriented polypropylene film/oriented polypropylene film);
2. BOPP/CPP-met. (biaxially oriented polypropylene film/oriented polypropylene surface metallized film);
3. BOPP/OPP-Chem (biaxial oriented polypropylene film/oriented polypropylene pearl film);
4. BOPP/PE (biaxially oriented polypropylene film/polyethylene).

Given the dependence of experimental polymeric materials on the process of ink interaction, pressure and printing speed, the study of the nature of ink with changing parameters aroused interest in changing the optical density during printing. The main purpose of this study is to search for regularities in the influence of the speed and pressure of printing equipment on the quality of printed products, to identify new approaches to improving the printing properties of the print.

It should be noted that each printing method, printed materials and description of the printing process and their results are unique. They are, of course, closely related to the printed materials (resin and ink) and the parameters of the printing process. Therefore, one of the most important tasks is to solve practical problems of improving the properties of printing equipment and printed products.

During the study, a statistical analysis was carried out to calculate the optical density of the printed dye layer on the sample surface and to estimate the thickness of the dye layer on the experimental polymer surfaces.

3 Results

The optimization parameter of y-coefficient of optical density of non-absorbent materials is significantly influenced by the following factors:

$X_1$—pressure $p$, MPa; $X_2$—speed $v$, m/min.

The selected variation intervals and factor levels are shown in Tables 1-4.

Table 1. Variation intervals and factor levels.

<table>
<thead>
<tr>
<th>Factors</th>
<th>Code designations</th>
<th>Variation intervals</th>
<th>factor levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure $p$, MPa</td>
<td>$X_1$</td>
<td>0.05</td>
<td>Upper +1</td>
</tr>
<tr>
<td>speed $v$, m/min</td>
<td>$X_2$</td>
<td>5</td>
<td>160</td>
</tr>
</tbody>
</table>

Table 2. The matrix planning and experiment results.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>$X_0$</th>
<th>$X_1$</th>
<th>$X_2$</th>
<th>$X_1X_2$</th>
<th>$Y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>1.04</td>
</tr>
<tr>
<td>2</td>
<td>+</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>1.10</td>
</tr>
<tr>
<td>3</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>1.15</td>
</tr>
<tr>
<td>4</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>1.03</td>
</tr>
</tbody>
</table>
The planning of the experiment was carried out for two areas of the response surface, when the upper factors, for example, the speed \( v \), vary in a narrow (150...160 m/min) and in a wide range (180...230 m/min). The intervals of pressure, respectively, is \( p = 0.3...0.4 \) MPa and \( p = 0.5...0.75 \) MPa.

This approach, when conducting experiments, allows estimating, through the regression equation, the local area of the response surface described by the optimization parameter and obtaining directions for the fastest achievement of the optimum area.

The processing of the results of the experiment in the absence of duplication of experiments is carried out in the following sequence:

1. To calculate the dispersion \( S^2_y \) and conducting the experiment, several parallel experiments are performed at the zero point (in the centre of the plan). According to the results of experiments in the centre of the plan, the dispersion experiment \( S^2_y \) is calculated repetitively.

\[
S^2_y = \frac{1}{n_0 - 1} \left[ \sum_{u=1}^{n_0} (y_u - \bar{y})^2 \right] \quad (1)
\]

Where: 
- \( n_0 \) - number of parallel experiments at the zero point;
- \( y_u \) - optimization parameter value in \( u \) experiment;
- \( \bar{y} \) - arithmetic mean value of the optimization parameter in \( n_0 \) parallel experiments.

\[
S^2_y = \frac{1}{3 - 1} [(1,028 - 1,033)^2 + (1,032 - 1,033)^2 + (1,038 - 1,033)^2] = 0.0000255
\]

**Table 3.** Variation intervals and factor levels.

<table>
<thead>
<tr>
<th>Factors</th>
<th>Code designations</th>
<th>Variation intervals</th>
<th>Factor levels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure ( p ), MPa</td>
<td>( X_1 )</td>
<td>0.125</td>
<td>0.75</td>
</tr>
<tr>
<td>Speed ( v ), m/min</td>
<td>( X_2 )</td>
<td>25</td>
<td>230</td>
</tr>
</tbody>
</table>

**Table 4.** Matrix planning and experiment results.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>( X_0 )</th>
<th>( X_1 )</th>
<th>( X_2 )</th>
<th>( X_1 X_2 )</th>
<th>( Y )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>+</td>
<td>0.93</td>
</tr>
<tr>
<td>2</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>1.12</td>
</tr>
<tr>
<td>3</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>1.10</td>
</tr>
<tr>
<td>4</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>+</td>
<td>1.02</td>
</tr>
</tbody>
</table>

2. According to the result of the experiment, the coefficient of the model is calculated. The indicator \( b_0 \) is determined by the formula:
The regression coefficients characterising linear effects are calculated by the formula:

\[ b_i = \frac{1}{N} \sum_{j=1}^{N} x_{ij} y_j \]  

(3)

\[ b_1 = \frac{1}{4} (-1,04 + 1,10 - 1,15 + 1,03) = -0,015; \quad b_2 = 0,01 \]

Regression coefficients characterising the effects of interaction:

\[ b_{i l} = \frac{1}{N} \sum_{j=1}^{N} x_{ij} x_{lj} y_j \]  

(4)

Where:  
\( i, l \) - numbers of factors;  
\( j \) - the number of the row or experiment in the planning matrix;  
\( y_j \) - optimization parameter values in \( j \)-experiment;  
\( x_{ij}, x_{lj} \) - coded values (±1) of factors \( i \) and \( l \) in the \( j \)-experiment.

\[ b_{12} = \frac{1}{4} (1,04 - 1,10 - 1,15 + 1,03) = -0,045; \]

3. Checking the statistical significance of the coefficients of the regression equation. The significance of the coefficients was checked by comparing the absolute value of the coefficient with a confidence interval. To determine the confidence interval, we calculate the dispersion of the regression coefficients by the formula below:

\[ S^2\{b_i\} = \frac{1}{N} S^2_y \]  

(5)

Where:  
\( S^2\{b_i\} \) - dispersion of the regression \( i \)-coefficient;  
\( N \) - the number of rows or experiments in the matrix.

\[ S^2\{b_1\} = \frac{1}{4} \cdot 0,0000255 = 0,000006375 \]

Errors in determining the regression \( i \)-coefficient;

\[ S\{b_1\} = \pm \sqrt{S^2\{b_1\}} \]  

(6)

\[ S\{b_1\} = \pm 0,0025 \]

The confidence interval \( \Delta b_i \) is found by the formula:

\[ \Delta b_i = \pm t_r S\{b_i\} \]  

(7)
\( t_T \) - is the tabular value of the criterion with the accepted levels of significance and the number of degrees of freedom \( f \), with which the dispersion \( S_y^2 \) is determined.

The values of the \( t \)-criteria for the significance level adopted at the 5% level and the number of degrees of freedom [3]:

\[
f = n_0 - 1 = 3 - 1 = 2 \quad \text{equal} \quad t_T = 4.3;
\]
\[
\Delta b_i = \pm 4.3 \cdot 0.0025 = \pm 0.01075
\]

Comparing all the values of the regression coefficients in absolute value with the confidence interval, it can be concluded that they can be considered statistically significant. Thus, we can see a model in the form of a polygon of the first degree.

\[
y = 1.08 - 0.015x_1 - 0.045x_1x_2 \quad (8)
\]
Equation (8) represents the regression equation with coded variables.

4. Determine the dispersion \( S_{ad}^2 \) of adequacy by the formula:

\[
S_{ad}^2 = \frac{\sum_{j=1}^{N}(y_j - \bar{y}_j)^2}{f} = \frac{\sum_{j=1}^{N}(y_j - \hat{y}_j)^2}{N - (k + l)} \quad (9)
\]

Where:
- \( y_j \) - is the observed value of the optimization parameter in the j-experiment;
- \( \hat{y}_j \) - is value of the optimization parameter calculated by the model for the conditions of the j-experiment;
- \( f \) - is the number of degrees of freedom, which for a linear model are determined by the given formula below:

\[
f = N - (k + 1) = 4 - (2 + 1) = 1
\]

Where: \( k \) - is a number of factors.

\[
S_{ad}^2 = \frac{(1.04 - 1.05)^2 + (1.1 - 1.11)^2 + (1.15 - 1.14)^2 + (1.03 - 1.02)^2}{4 - (2 + 1)} = 0.0004
\]

5. Checking the adequacy of the model according to Fisher's \( F \)-criteria. Let us determine the calculated value of the criteria \( F_p \):

\[
F_p = \frac{S_{ad}^2}{S_y^2} = \frac{0.0004}{0.0000255} = 15.69
\]

The table values of the \( F_T \)-criteria at a 5% significance level and the number of degrees of freedom for the numerator 1 and for the denominator 2 is equal 18.5, \( F_p < F_T \). Therefore, the model is adequate.

The processing of the results of a repeated experiment (Tables 3 and 4) in the absence of duplication was carried out in the same sequence according to the formulas (1), (7) and (9).

1. Dispersion \( S_y^2 \) of the reproducibility of the experiment.

\[
S_y^2 = \frac{1}{3 - 1}[(1,025 - 1,035)^2 + (1,035 - 1,035)^2 + (1,045 - 1,035)^2] = 0.001
\]
2. Model’s coefficient

\[ b_0 = 1.0425; \quad b_1 = 0.0275; \quad b_2 = 0.0175; \quad b_{12} = -0.0675; \]

3. Checking the statistical significance of the coefficients of the regression equation. Dispersion of regression coefficients:

\[ S^2 \{b_i\} = \frac{1}{4} \cdot 0.0001 = 0.000025 \]

Error in determining the i-regression coefficient:

\[ S\{b_i\} = \pm \sqrt{0.000025} = \pm 0.005 \]

Confidence interval \( \Delta b_i \):

\[ \Delta b_i = \pm 4.3 \cdot 0.005 = \pm 0.0215 \]

Regression equation with coded variables:

\[ y = 1.0425 + 0.0275 x_1 - 0.0675 x_1 x_2 \quad (10) \]

4. Dispersion of adequacy:

\[ S_{ad}^2 = \frac{(10.93 - 0.94751)^2 + (1.12 - 1.1375)^2 + (1.10 - 1.0825)^2 + (1.02 - 1.0025)^2}{4 - (2 + 1)} \]

\[ = 0.001225 \]

5. Checking the adequacy of the model according to Fisher's \( F \) -criteria:

\[ F_p = \frac{0.001225}{0.0001} = 12.25 \]

\[ F_T = 18.5; \quad F_p < F_T \]

Thus, the model is adequate.

4 Discussion

The analysis of equations (8) and (10) shows that the degree of influence of the pair interaction \( X_1X_2 \) is much greater, respectively, 3 and 2.45 times, than the factor \( X_1 \) -is the pressure \( p \) (MPa).

Graphical interpretation of the dependences of the optical density coefficient on pressure \( p \) at different speeds \( v \) (Figures 1 and 2) showed that the combination of \( p = 0.3 \ldots 0.4 \) MPa at \( v = 150 \text{ m/min} \) and \( p = 0.5 \ldots 0.75 \) MPa at \( v = 180 \text{ m/min} \) leads to an increase in the coefficient \( D \).

The combination of pressures \( p = 0.3 \ldots 0.4 \) MPa at \( v = 160 \text{ m/min} \) and \( p = 0.5 \ldots 0.75 \) MPa at \( v = 230 \text{ m/min} \) contributes to a decrease in the optical density coefficient, respectively, 10.4 and 7.3%.
Thus, the pressure $p=0.75$ MPa and $v=180$ m/min can be considered a rational mode.

Fig. 1. Dependence of the optical density coefficient $D$ of non-absorbent materials on pressure $p$: 1- $v = 150$ m/min; 2- $v = 160$ m/min.

Fig. 2. Dependence of the coefficient of optical density $D$ of non-absorbent materials on pressure $p$: 1- $v = 180$ m/min; 2- $v = 230$ m/min.

In connection with the increase in printing speed, the time factor is of great interest. The speed and degree of transfer of printing ink on a polymer material largely depends on the kinetics of ink absorption, which in turn is determined by capillary and molecular interactions in interacting systems.

5 Conclusions

Experiments show that despite the increase in speed, the optical density of the printed image increases, with an increase in the speed of the printing equipment, the amount of ink transferred to the printed material and, consequently, the optical density of the printed image also increases.

As the pressure increases under a high-speed dynamic load, the nature of the deformation movement of the printed material changes. The short contact time is not enough to force the
air out of the ink print, so the ink only covers the surface of the printed material, not entering the narrow groove. In this case, the ink layer can be quickly fixed, and even when the ink transfers from the form to the printed material, the saturation of the image will be much higher.

It is shown that with an increase in pressure from 0.5 to 0.8 MPa, the amount of paint transferred from the form to the polymer surface increases by 10-15%. It has been established that the optical properties of printing on experimental polymeric materials under constant printing conditions are determined by the internal and external structure, as well as the molecular nature of the printed material. Thus, it has been experimentally confirmed that the optical density of continuous sections of the image depends on both pressure and velocity.

References