Modeling with Fuzzy Logic the Migration Capacity of UV-ink Components as a Factor of Potentially Harmful Pollution of Packaging

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Abstract

The implementation of UV-technologies has revealed problems associated with the migration of harmful components of the ink layer to the back of the packaging in contact with the packaged products. The reason for this migration is the incomplete reaction of the UV-ink components due to a decrease in the intensity of UV-radiation, the mismatch between the absorption spectrum of the photoinitiator and the spectrum of the UV-source and the inhibitory effect of oxygen. It has been established that the decay products of photoinitiators, which occupy the third position in terms of concentration content in the ink composition, have a potential ability to migrate. To prevent such migration, polymerized photoinitiators have been developed that differ from conventional ones by higher molecular weight. Accordingly, a study of the effect of the photopolymerization degree of UV-ink on the presence of residual odor, as a direct characteristic of the ability of ink components to migrate has been done. It has been found that at the photopolymerization degree of 84%, the average value of the residual odor level is 4 points, and at the photopolymerization degree of 96%, it is 2.8 points. Using the obtained data on the presence of residual odor and the data on the influence of molecular weight of photoinitiators, a knowledge base has been formed with the condition "if-then", a logical scheme has been formed and fuzzy logical equations of influence of established factors on the migration capacity of UV-ink have been constructed. The establishment of a universal set and evaluation terms has made it possible to form a quantitative indicator of migration of UV-ink components. The formed fuzzy knowledge base has been checked when modeling with the help of the Fuzzy Logic Toolbox system of the Matlab technological calculation environment according to Mamdani principle, using the method "Center of gravity" for the dephasification operation. The suggested method of calculating the migration capacity of UV-inks has made it possible to construct a two-factor forecasting model.

Keywords

UV-inks, packaging, migration, fizzy logic, linguistic variables, model.

1. Introduction

The development of photopolymerizable inks (UV-inks) has given the impetus to the improvement of printing processes. Instant drying of imprints under the influence of actinic UV-radiation has made it possible to further process them without additional technological downtime, and the imprints

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themselves have high optical and operational performance parameters [1]. The application of UV-inks has raised the screen printing method to a new level, such inks are stable in the printing process, and their drying inability on the printing plate has allowed its "in line" integration in machines with other printing methods. The implementation of such innovations has revealed problems associated with the harmfulness of this technology, namely the need to eliminate ozone gas, which is formed due to the action of UV-light with a spectrum of 250 nm. The development of UV-LED systems of light sources with a clearly concentrated spectrum in the sensitivity zone of the photoinitiators (PI) of the ink composition managed to avoid such a disadvantage. Another disadvantage of UV-technology is the inhibitory effect of air oxygen on the process of photoinitiated radical photopolymerization. The decrease in the intensity of UV-radiation, the mismatch between the absorption spectrum of the photoinitiator and the spectrum of the UV-source and the inhibitory effect of oxygen lead to a decrease in the photopolymerization degree of the ink layer and as a consequence the residual odor, characteristic of acrylate systems and the possible migration of unreacted ink components to the reverse side of the packaging, which is especially dangerous for the packaging of food and pharmaceutical products.

In the recent past, the detection of residues of the photoinitiator Isopropyl Thioxantone in packaged products [2, 3], despite the lack of results of toxicological examination, led to the review of the composite content of UV-inks and its exclusion from production by manufacturers. In general, a number of regulatory documents have been adopted, which concern both the restriction of the concentration content and the prohibition of some photoinitiators and monomer compounds in the production of UV-inks for the food packaging production [4, 5, 6].

2. Literature review

In the technological process of packaging printing and manufacturing, as well as during its operation, the following options of migration of printing ink components are possible (Fig. 1): the contact of the front and back of the imprints, evaporation and penetration (diffusion) [7].

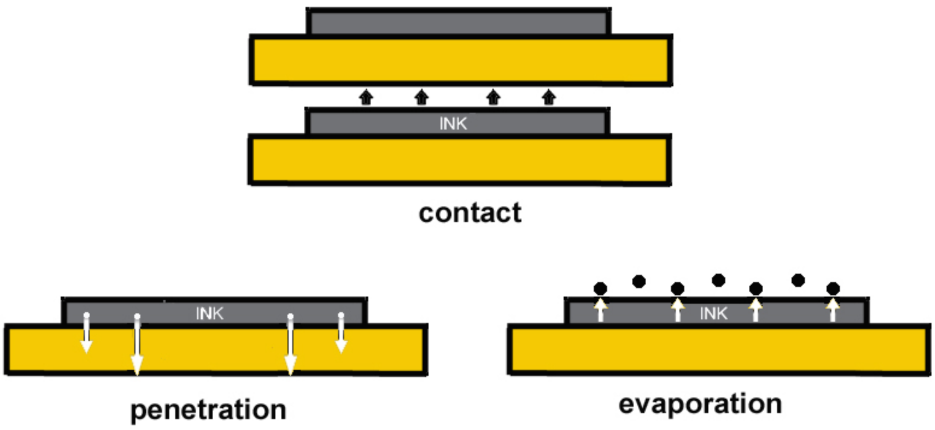


Figure 1: Options of possible migration of UV-ink components in the process of packaging printing and operation

Manufacturers of UV-inks and their chemical components have found that decay products of photoinitiators which occupy the third position in terms of concentration in the ink composition have the potential for migration [8]. To prevent such migration, polymerized photoinitiators and synergistic impurities have been developed that differ from conventional ones by higher molecular weight. For example, if conventional photoinitiators are characterized by the molecular weight of 160-400 g/mol, the polymerized ones have 700-1200 g/mol.

Therefore, forecasting the effect of the molecular weight of the photoinitiator and the polymerization degree of the UV-ink layer of on the migration amount of its components is relevant. In the forecasting area, there are publications related to the application of fuzzy logic to ensure the quality of technological processes [9, 10], comprehensive quality assessment of flexographic imprints [11], as well as forecasting the book quality and design [12].

To develop a model for forecasting the potential harmful contamination of packaging during the migration of UV-ink components with a radical photoinitiated polymerization mechanism.

3. Methods

The development of systems capable of adequately reproducing human reasoning requires a mathematical apparatus that would interpret ambiguous statements into the language of clear and formal mathematical formulas. This principle was introduced by Latfi Zadeh, who developed the basics of fuzzy logic and introduced the concept of a universal set for a particular problem area [13]. Fuzzy logic is the logic that operates with linguistic variables using the rules that are understandable to humans and close to ordinary spoken language in structure. The advantage of a system with fuzzy logic is the ability to operate with fuzzy input data and combine them with the results of experimental studies. In particular, the fuzzy form is characterized by an organoleptic test [14], in which the odor is evaluated in points according to the judgments of the expert group within the assessment limits: no odor – 0 points, very strong odor – 4 points.

To determine the effect of the photopolymerization degree on the migration capacity of the ink layer, a model photopolymerizable UV-ink binder was developed based on epoxyacrylate oligomer and photoinitiator 1-hydroxycyclohexyl-phenyl ketone (Omnirad 184, IGM Resin). UV-ink binder was applied with the thickness of 10 μm on the surface of coated paper, weighing 200 g/m^2 of Magno Gloss brand, (Sappi Group) and was irradiated with a UV-lamp DRT-400 with UV intensity of 95 W/m^2. The polymerization degree of the UV-ink binder at different irradiation times was evaluated by the method of determining the gel-sol fraction [15].

The migration of the components of UV-printing inks depends primarily on the molecular weight of its components and the photopolymerization degree of the applied ink layer. Accordingly, the migration amount of the UV ink components is defined as:

$$M_K = f(M, P), \tag{1}$$

where M is a linguistic valuable which characterizes the molecular weight of the photoinitiator;
P is a linguistic valuable which characterizes the photopolymerization degree of the ink layer.

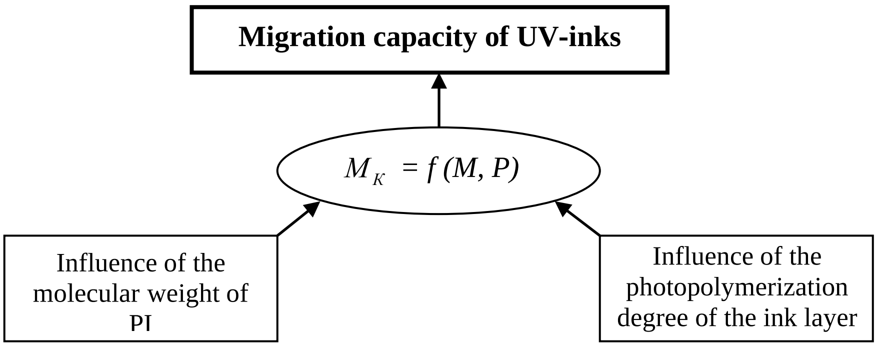


Figure 2: Example Logical block diagram of the conclusion about the influence of the molecular weight of the components and the photopolymerization degree of the ink on its migration capacity

According to the results of expert judgments and experimental studies, one will form a block diagram of a logical conclusion about the influence of the molecular weight of the components and the photopolymerization degree of the ink on its migration capacity (Fig. 2).

One can evaluate the values of linguistic variables using a system of qualitative concepts that make up the corresponding fuzzy set, i.e. some property of the factor, which is considered as a linguistic term. For our membership functions, you can apply the division into three members of each input variable with a symmetric Gaussian membership function:

$$\mu(x) = e^{-\frac{(x-h)^2}{2c^2}}, \tag{2}$$

where x is an element of a universal set; h is a parameter of a membership function (maximum coordinate); c is a parameter of a membership function (concentration ratio).

4. Results and Conclusions

Selected samples with a certain photopolymerization degree were simultaneously evaluated by the odor amount as a characteristic of the migration potential of UV-ink. The results of the study are shown in Table 1.

Table 1
Results of determining the residual odor of photopolymerizable UV-ink binder

№	Photopolymerization degree, %	Questionnaire of answers of one expert		The average score of the survey of 5 experts, points
		Questionnaire of answers of one expert	Odor assessment, points	
1	84	Strong odor	4	4
2	87	Strong odor	4	4
3	90	Moderate to strong odor	3	3,2
4	93	Moderate odor	2	3,0
5	96	Moderate odor	2	2,8

Linguistic variables, on which the migration capacity of ink components and assessment terms depend, are presented in Table 2.

Table 2
Linguistic variables of the influence on the migration capacity of UV-ink components

Name of the valuable	Universal set	Assessment terms
Molecular weight of the photoinitiator	200-1000 g/mol	low medium high
Photopolymerization degree of the ink layer 84-96 %	84-96 %	low medium high

Based on the results of the influence of the molecular weight of the photoinitiator [16] and the photopolymerization degree of the ink layer (IL) on migration, one can construct membership functions. Accordingly, the value of the parameter "Molecular weight of PI" is determined on the universal set: u_1 = 200 g/mol; u_2 = 400 g/mol; u_3 = 600 g/mol; u_4 = 800 g/mol; u_5 = 1000 g/mol.

For a linguistic assessment of this parameter, one can use a set of fuzzy terms: *M (x)* = <low, medium, high>. In accordance with these terms, one obtains the membership functions of the linguistic variable "Molecular weight of PI" (Fig. 3, a).

For the variable "Photopolymerization degree of IL", one can set the universal set: u_1 = 84% ; u_2 = 87%; u_3 = 90%; u_4 = 93%; u_5 = 96%. For a linguistic assessment of the variable, one uses a set of fuzzy terms: *P(y)* = <low, medium, high>. Therefore, taking into account the results of determining the residual odor, for the indicator "Photopolymerization degree of IL" in relation to these terms, one can construct membership functions (Fig. 3, b).

One can form a fuzzy knowledge base on the selected parameters of the quality of the digitization process:

1. For the term “low” migration:

- if the molecular weight of PI is "high", the photopolymerization degree of IL is "high", the migration is "low"

or

- if the molecular weight of PI is "high", the photopolymerization degree of IL is "medium", the migration is "low".

2. For the term “medium” migration:

- if the molecular weight of PI is "high", the photopolymerization degree of IL is "low", the migration is "medium"

or

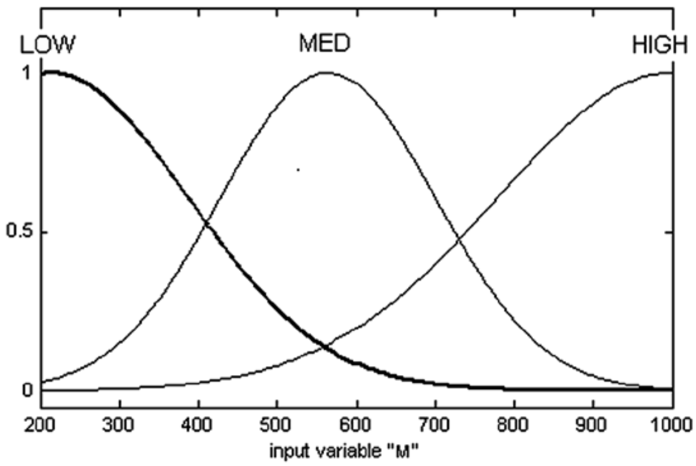
- if the molecular weight of PI is "medium", the photopolymerization degree of IL is "medium", then migration is "medium".

3. For the term “high” migration:

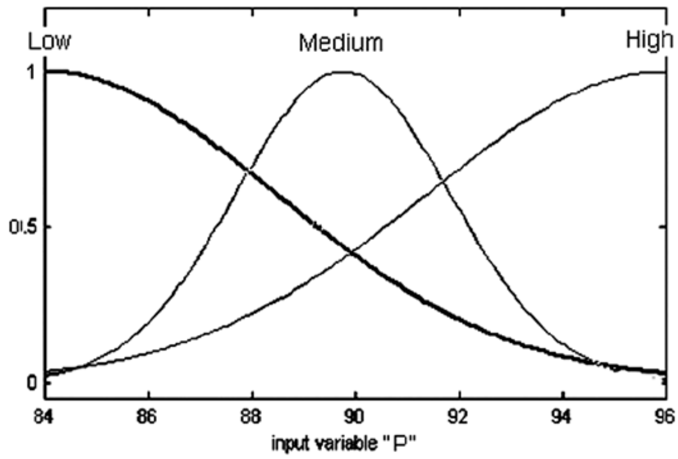
- if the molecular weight of PI is "low", the photopolymerization degree of IL is "low", then the migration is "high"

or

- if the molecular weight of PI is "medium", the photopolymerization degree of IL is "low", then migration is "high".



a



b

Figure 3: Example Logical block diagram of the conclusion about the influence of the molecular weight (a) and photopolymerization degree (b)

Logical equations for forecasting the migration amount of UV-ink components are:

$$\mu^{l} = \mu^{h}(x) \wedge \mu^{h}(y) \vee \mu^{h}(x) \wedge \mu^{m}(y), \quad (3)$$

$$\mu^{m} = \mu^{h}(x) \wedge \mu^{l}(y) \vee \mu^{m}(x) \wedge \mu^{m}(y), \quad (4)$$

$$\mu^{h} = \mu^{l}(x) \wedge \mu^{l}(y) \vee \mu^{m}(x) \wedge \mu^{\text{н}}(y). \quad (5)$$

The notations   and   are the operations of determining the minimum and maximum in logical equations. Using the membership functions and substituting the membership degrees into the system of fuzzy logical equations, one can forecast the migration options of the ink components

The formed fuzzy knowledge base has been checked when modelling with the help of the Fuzzy Logic Toolbox system of the Matlab technological calculation environment according to Mamdani principle [17, 18, 19] (Fig. 4). To carry out the defuzzyfication operation by the "center of gravity" method [20], one can set the upper and lower limits of the quality of the process Q: lower – 1 unit, upper – 10 units. After the defuzzification of the obtained fuzzy values of the process, one obtains a quantitative assessment of the migration amount of UV-ink components.

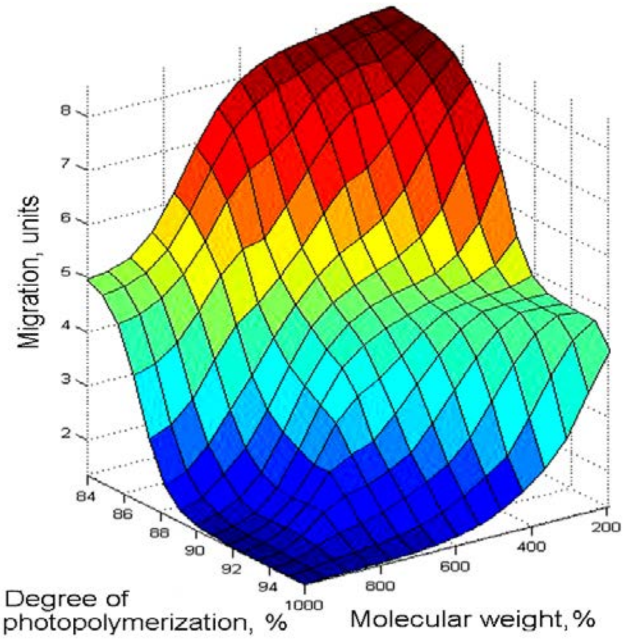


Figure 4: Model of influence of the molecular weight of the photoinitiator and the photopolymerization degree of the ink layer on the migration of UV-ink components

According to the formed logical equations and the constructed model, several variants of the dependence of the migration capacity of the UV-ink components on its degree of photopolymerization and the molecular weight of the photoinitiator are calculated (Table 3).

Table 3

Variants of the dependence of the migration capacity of the UV-ink components

Molecular weight of the photoinitiator, g/mol	Photopolymerization degree of the ink layer , %	Migration capacity, un
200	84	8,42
200	90	5,02
200	96	5,0
600	84	7,13
600	90	4,78
600	96	2,31
1000	84	4,02
1000	90	1,52
1000	96	1,4

The simulation results have shown the possibilities of applying the developed knowledge base for forecasting assessment of the migration capacity of UV-ink components.

Therefore, the influence of the photopolymerization degree of the UV-composition on the value of the residual odor as a direct characteristic of the migration capacity of unreacted components has been established in the paper. Using data on the influence of the photopolymerization degree and the molecular weight of the photoinitiator, the analysis has been performed using fuzzy expert-linguistic information and the rule "if-then", which allowed one to obtain fuzzy logical equations of the influence of linguistic variables on migration capacity and, accordingly, to quantify it. The suggested calculation of the migration capacity of UV-ink components allows the development of a simulation model for forecasting the possible harmful contamination of packaging.

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