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Synthesis of flexible polyurethane foam for applications in planar orthosis using the response surface methodology

Síntesis de espuma de poliuretano flexible para aplicaciones en ortesis planares utilizando la metodología de superficie de respuesta

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Abstract

In this work, the process for the formulation of flexible polyurethane foam is presented following a design of experiments for mixtures. The proportion of polyol, diisocyanate, and crosslinker was considered as factors. The response variables considered were foaming time and reaction temperature. The result of the experiments showed that there is an area where the foam formulation is better. This zone is closed with 5% crosslinker, 50% polyol, and 45% diisocyanate, in this formulation denser foams with more uniform bubbles were obtained.

Polyurethane foam, Polyol, Diisocyanate

Resumen

En el presente trabajo se presenta el proceso para la formulación de una espuma de poliuretano flexible siguiendo un diseño de experimentos para mezclas. Se consideraron como factores la proporción de poliol, diisocianato y reticulante. Las variables de respuesta consideradas fueron el tiempo de espumado y la temperatura de reacción. El resultado de los experimentos mostró que existe una zona donde la formulación de la espuma es mejor, esta zona está cerana al 5% de reticulante, 50% de poliol y 45% de disocianato, en esta formulación se obtuvieron espumas más densas con burbujas más uniformes.

Espuma de poliuretano, Poliol, Disocianato

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Introduction

Polyurethane foams are polymers with a high range of applications, such as packaging, automotive industry, electronics, footwear, construction, etc [1]. The formation of polyurethane foam is carried out when an isocyanate reacts with a polyol to form a urethane functional group, as shown in Figure 1.

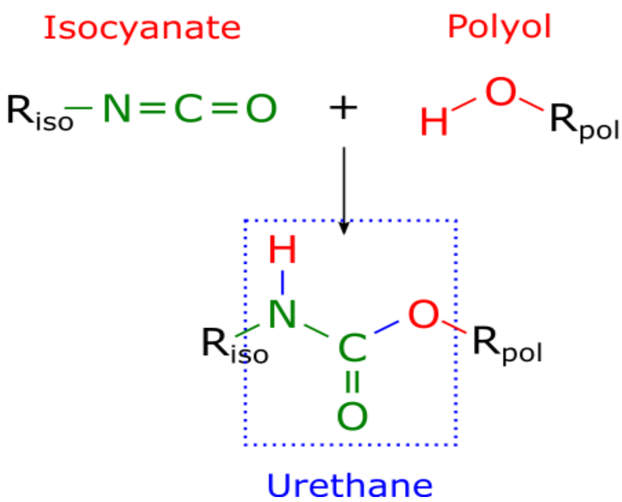

Figure 1 Reaction between isocyanate and polyol to form the urethane functional group
Source: own work

Experimental design

To optimize the formulation of a chemical mixture, it is necessary to carry out a design of experiments for the mixtures. An important property of the design of experiments is the quantification of the change due to a response variable [3]. The design experiment for the mixture has some additional restrictions such as the sum of the proportions of all the factors is always equal to the total mixture, Eq (1).

$$x_1 + x_2 + \cdots + x_n = 1 \quad (1)$$

To model the response surface it is necessary to adjust the experimental points to an already known mathematical model [4].

$$R(y) = \sum_{k=1}^{n} \beta_k \, x_k \quad (2)$$

$$R(y) = \sum_{k=1}^{n} \beta_k \, x_k + \sum \sum_{k<j}^{n} \beta_{kj} \, x_k \, x_j \quad (3)$$

$$R(y) = \sum_{k=1}^{n} \beta_k \, x_k + \sum \sum_{k<j}^{n} \beta_{kj} \, x_k \, x_j + \sum \sum_{k<j<m}^{n} \sum \beta_{kjm} \, x_k \, x_j \, x_m \quad (4)$$

In equations 2 to 4, the parameter β_k represents the linear contribution of each of the factors to the total mixture, the parameter β_{kj} represents the interaction of two factors after the final mixture, this can be synergistic, if the response improves, or antagonistic if the response worsens. The parameter β_{kjm} represents the interaction between of all components of the mixture.

Methodology

A proportion of polyol was mixed with diisocyanate as shown in the design of experiments in Table 1, the precursors were vigorously mixed with a wooden mixer for 3 seconds. then the reaction temperature was measured and the time it took to start foaming.

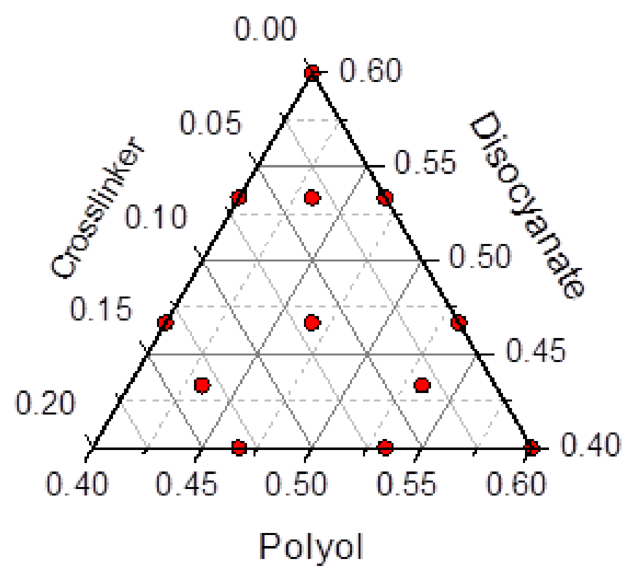

Figure 2 Ternary diagram of the feasible zone in the design of experiments, the red numbers indicate the ID of the experiment
Source: own work

The constraint for this experiment was 40 to 60% polyol, 40 to 60% diisocyanate, and 0 to 20% crosslinker. Figure 2 shows the experiments within the feasible zone. All experiments were carried out at room temperature, first activating the polyol with the crosslinker, and then adding the active polyol mixture to the diisocyanate.

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Test	Polyol	Diisocyanate	Crosslinker
1	0.600	0.400	0.000
2	0.467	0.400	0.133
3	0.533	0.467	0.000
4	0.433	0.533	0.033
5	0.533	0.400	0.067
6	0.467	0.467	0.067
7	0.467	0.467	0.067
8	0.400	0.400	0.200
9	0.400	0.600	0.000
10	0.400	0.467	0.133
11	0.400	0.533	0.067
12	0.433	0.433	0.133
13	0.533	0.433	0.033
14	0.467	0.533	0.000

Table 1 Composition of the mixture following a design of experiments for mixtures
Source: own work [Excel]

Results

In each experiment, the room temperature and the temperature when the foaming reaction started were measured. Figure 3a shows the preparation of the mixture in the first block of experiments. The formation of cream is observed before the reaction and the start of the foaming reaction. In Figure 3b, the foams formed can be observed, considering that the foaming speed is correlated with the porosity of the material. It can also be observed that at a higher reaction temperature, there is a material with larger bubbles.

Figure 3 a) Experiment where the measurement of reaction temperature and foaming time was carried out b) experiment selection with better foaming speed control
Source: own work

Tes t	Foaming Time (s)	Reaction Temperature (°C)
1	14	40.3
2	5	60.4
3	24	30.8
4	19	45.8
5	7	55.2
6	8	53.1
7	6	54.8
8	5	61.2
9	31	40.1
10	5	60.7
11	6	51.9
12	5	59.9
13	17	40.6
14	27	33.4

Table 2 Result of the measurement of foaming time and reaction temperature
Source: own work [Excel]

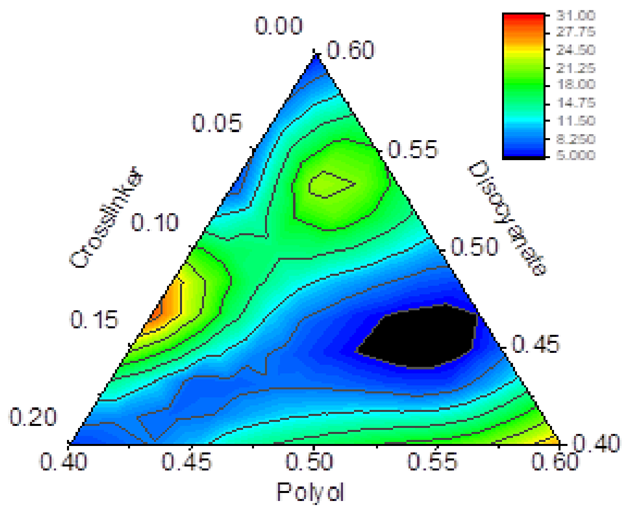

Figure 4 Ternary diagram of the feasible zone in the design of experiments, the red numbers indicate the ID of the experiment
Source: own work

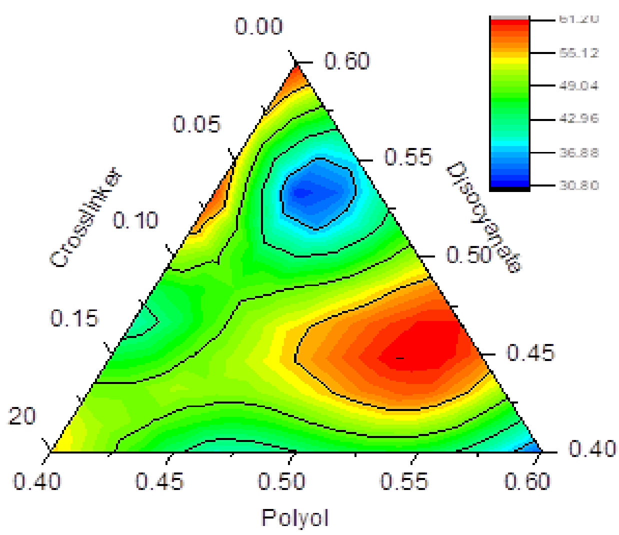

Figure 5 Ternary diagram of the feasible zone in the design of experiments, the red numbers indicate the ID of the experiment
Source: own work

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Figures 4 and 5 represent the best response surface with the data obtained fitting to equation 5 correspondings to a special cubic model. In Figure 4 the black zone can be observed, which indicates that the foaming reaction time is short, while in Figure 5 it is observed in that same zone that the reaction temperatures are higher. Also, in that area, the best polyurethane foams were found.

Conclusions

It was possible to formulate polyurethane foams employing a design of experiments for mixtures, finding that the foams with a percentage close to 5% of crosslinker, 50% polyol and 45% diisocyanate. In that area it was found that the reaction temperature is high, and the foaming time is short, it was also seen that the foams in this area had a better appearance.

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