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# **Book of Abstracts**

## T2P11 – MIGRATION KINETICS OF TWO THIOXANTHONE PHOTOINITIATORS INTO FOOD SIMULANTS

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#### • Introduction

Since 2005, when the Italian authorities reported a case of isopropylthioxanthone (ITX) in milk, the food safety authorities labeled the photoinitiators as one of the biggest food safety concerns. The ITX was the first photoinitiator notified by RASFF; however, the presence of more photoinitiators in foodstuffs came swiftly, as it was the case of 2,4-diethylthioxanthone (DETX), another thioxanthone (1). Thioxanthones are one of the two biggest groups of type II photoinitiators (the other is the benzophenones), and they are commonly used alone or with other photoinitiators in food packaging, being extensively used due to not produce photo-yellowing and produce very-low migration rates (2).

The aim of this work is to study the migration of the thioxanthone photoinitiators into the food simulants proposed by the European Regulation 10/2011 (3) where these photoinitiators are soluble (50 and 95% ethanol (v/v)). The diffusion coefficient ( $D_e$ ), one of the parameters of the migration processes was calculated according to the Crank mathematical solutions based on Fick's second law (4). The effect of the temperature on the diffusion was study applying Arrhenius equation.

#### • Materials and methods

The photoinitiators selected were: ITX (CAS No. 5495-84-1) and DETX (CAS No. 82799-44-8). The food simulants were performed mixing ethanol (absolute for analysis) with distilled water. As source, LDPE was selected and the photoinitiators were included separately into two LDPE matrixes by extrusion.

The methodology was as follows: sheets of each obtained film were immersed in tubes filled with the food simulant, protected from the light. The migration kinetics were performed by duplicate at three different temperatures: 4, 20 and 40 °C. An aliquot of the food simulant was removed from each sample at preset times and they were injected in an HPLC-DAD system, in order to quantify the migrant released at 256 nm. The chromatographic method used was the same used by Lago et al. (5).

The experimental data were exported to Solver function of Microsoft<sup>®</sup> Excel 2010 software, to determine the diffusion coefficients of ITX and DETX in each food simulant and temperature. Also, the data obtained was applied to the Arrhenius equation.

#### • Results and Discussion

The diffusion coefficients obtained for these two photoinitiators are of the same order of magnitude at each temperature, being a little faster ITX than DETX. Taking 95% ethanol (v/v) as example, the  $D_e$  obtained for ITX ranged from 1.59E-10 at 4 °C to 6.14E-9 at 40 °C, in the case of DETX the values are slower (5.55E-11 at 4 °C to 3.97E-9 at 40 °C). This little difference could be explained by the smaller molecular weight of ITX, 254.35, in comparison with the DETX 268.37.

To determine the effect of the temperature in the process of migration, the  $D_e$  obtained were applied to the Arrhenius equation and the results are showed in Figure 1. As can be observed, the relation between the

 $D_e$  logarithm and the inverse of the temperature draws a straight line with good coefficients of determination (R<sup>2</sup> > 0.9760). With this good linearity results, the  $D_e$  of ITX and DETX can be calculated in the range of temperatures between 4 and 40  $^\circ$ C for these food simulants.

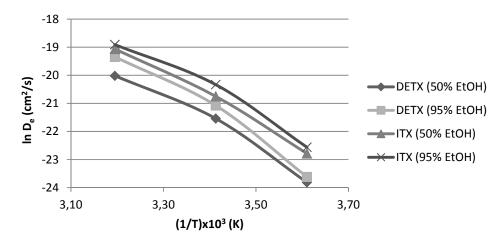


Figure 1 – ITX and DETX diffusion coefficients (De) linearity.

#### Conclusions

The obtained data provides reliable data of the ITX and DETX migration into foodstuffs. Also, the linearity obtained, with the application of the Arrhenius equation to the data obtained, provides accurate estimation of the diffusion coefficients in the range of temperatures worked.

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