Probabilistic Simulation of Children Exposure to Migrants from Packaging: Photoinitiators from Printing Inks

Carla Machado[1], Conceição Fernandes[1], Joel Pereira[2], Maria de Fátima Poças[2]

[1]Escola Superior Agrária, Instituto Politécnico de Bragança; Centro de Investigação de Montanha (CIMO), Bragança, Portugal

[2]Packaging Department, Biotechnology College, Portuguese Catholic University, Porto, Portugal

ABSTRACT

The present work presents an exercise to simulate exposure of Portuguese consumers to benzophenone, a photoinitiator used in packaging printing inks. The simulation model combined experimental data of benzophenone concentration found in packages collected from market and food consumption and packaging usage data obtained from a database. The model followed a probabilistic approach: the distribution of occurrence data was combined with food consumption data in a probabilistic simulation with the Monte Carlo sampling method. The values found indicate that benzophenone levels of exposure are of no health concern according to the tolerable daily intake defined by EFSA.

INTRODUCTION

Simulation modelling is recognised today as an important tool in different issues related to food safety risk assessment. There is an increasing interest in models that follow a probabilistic approach allowing for quantifying variability and uncertainty in the estimates, for example in exposure assessments of contaminants migrating from food packages is of increasing interest [1]. Stochastic models are represented by functions of probability distribution rather than single values for the model inputs and the outputs are also distributions of estimate values. They give quantitative information about both the range and the likelihood of possible estimate values [2].

Photoinitiators are substances used in the formulation of inks, particularly UV-cured inks that have a much shorter drying time than other inks. In the area of food packaging benzophenone (BZP) is a photoinitiator that have recently been re-evaluated [3]. Although ink is applied in the outer or in an intermediate layer of the packaging material, these ink components can migrate in to the food due to their volatility if there is no functional barrier and by set-off process. EFSA re-assessed the tolerable daily intake (TDI) on BZP and derived a new value of 0.03 mg/day. $Kg_{body\ weight}$ [3].

The work presented here is included in an on-going surveillance exercise to determine the BZP occurrence on paperboard packages and simulate the children's exposure to BZP with origin in paper and paperboard packaging. An exposure model was derived and the variability in the model inputs was propagated by a Monte Carlo simulation to estimate the probability distribution function of the exposure values.

MATERIAL AND METHODS

• Exposure model

Exposure of consumer to substances with origin in packaging systems can be expressed as [1]:

$$Exposure = Migration\ x\ Food\ Consumption \quad (1)$$

Where:

Migration represents the concentration of substance that, by transfer from the package, ends in the food;

Food Consumption represents the daily intake of food packaged in the system from which the migrant originated, or the amount of packaging used to pack the food consumed, depending on the units used in the migration term.

Concentration on the food was assumed to be the concentration that it would be achieved if the total amount of BZP found in the packages would migrate. In that case the concentration in the food can be derived from the concentration found in the packaging and the ratio of the packaging material weight to the weight of the contained food:

$$C_{Food} = C_{Pack} \cdot \frac{W_{Pack}}{W_{Food}} \quad (2)$$

Combining equation 1 and 2 gives:

$$E(mg_{BZP} / day.Kg_{bw}) = C_{Pack} \cdot \frac{W_{Pack}}{W_{Food}} (mg_{BZP} / Kg_{Food}).FW(Kg_{Food} / day.Kg_{bw}) \quad (3)$$

Where:

E represents the exposure to BZP

FW represents the amount of food packaged in paper and board consumed per day and per Kg_{bw}.

•Concentration of BZP in the packages

Foods (30) consumed by children and packaged in paper and board systems were purchased in one supermarket in Gaia, Portugal, in 2009 and 2010. The packaging materials were extracted with acetonitrile at 70ºC for 1 day or 40ºC for 2 days. The extracts were analysed by GC-MS.

•Ratio of the packaging material weight to the weight of the contained food

The database from MIGRAMODEL project [4] was used to provide data on the ratio of the packaging material weight to the weight of the contained food registered in the Portuguese market for paper and board packaging.

•Food consumption

The database from MIGRAMODEL project [4] was used to provide data on the amount of food in contact with paper and paperboard packages.

•Probabilistic analysis

The software Crystal Ball 7.2.2. (Decisioneering, Inc.) was used to fit the exposure model inputs as well as the model output to probability distributions functions by the maximum likelihood method. The goodness-of-fit was assessed by the Anderson-Darling (A-D) test. MC simulation was used as sampling method with 10 000 iterations.

RESULTS

• Input variables and parameters of functions

Table 1. Input variables for exposure model: BZP concentration in the packaging, ratio of packaging weight to food weight, daily intake of food.

	C_{BZP}, mg/Kg_{Pack}	W_{Pack}/W_{Food}	FW, $Kg_{Food}/day.Kg_{bw}$
Mean	2.61	0.136	0.017
Standard Error	0.47	0.010	0.001
Median	2.49	0.082	0.017
Standard Deviation	2.60	0.256	0.008
Sample Variance	6.76	0.065	0.000
Kurtosis	0.71	176.680	-0.260
Skewness	1.02	11.540	0.602
Range	9.39	4.591	0.031
Minimum	0.08	0.002	0.005
Maximum	9.47	4.593	0.036
Count	30	628	34

Table 2. Parameters of functions describing the distribution of values of the exposure model inputs.

Input	Distribution	Parameters
C_{BZP}, mg/Kg_{Pack}	Beta	α=0.9709 β=3.3840
W_{Pack}/W_{Food}	Lognormal	L=0 Mean=0.13 Stand. Dev.=0.19
FW, $Kg_{Food}/day.Kg_{bw}$	Lognormal	L=-0.01 Mean=0.02 Stand. Dev.=0.01

• Food consumption and ratio packaging weight/food weight

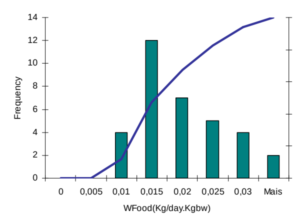

Figure 1. Distribution of consumer food consumption .

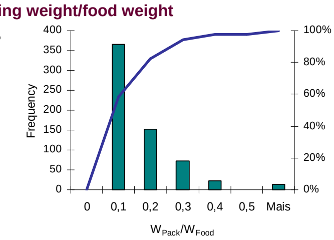

Figure 2. Distribution of values for Pack/Food weight ratio.

Table 1 presents the descriptive statistics for the concentration of BZP found in the cellulosic packages collected from the market and the data extracted from the MIGRAMODEL database required as inputs in the exposure model. The highest concentration values (9 mg/Kg) were found in boxes of cookies and cereal. The total food weight consumed per day and per consumer body weight averaged 0.017 $Kg_{food}/day.Kg_{bw}$ (Figure 1). From this total amount of food an average of 12% have been packaged in paper and board materials [5]. The ratio of packaging material to food weight (W_{Pack}/W_{Food}) presents an average value of 0.14 ranging from 0.002 up to 4.6 (Figure 2). Table 2 presents the results for the distribution functions fitting the input variables for the exposure model.

Figure 3 shows the simulated exposure of consumers to BZP migrating from paper and board packaging materials, obtained with equation 3 and running 10 000 iterations Monte Carlo. Results show mean exposure values 9.97E-4 $mgBZP/day.Kg_{bw}$ and maximum value of 3.1E-2 $mgBZP/day.Kg_{bw}$, indicating that the TDI value defined by EFSA is hardly achieved: the 99% percentile of consumers have simulated exposure values lower than 8.85E-3 $mgBZP/day.Kg_{bw}$. These results also indicate that additional efforts in refining the exposure estimates are not required in the present case.

• Simulated exposure of consumers to BZP

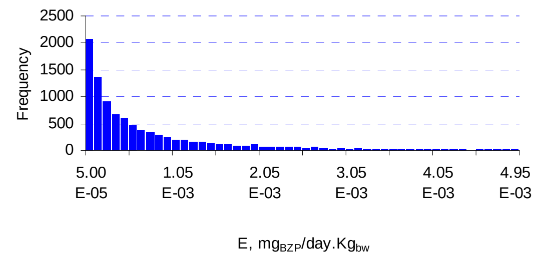

Figure 3. Simulated exposure to BZP.

CONCLUSIONS

Simulation models may be applied to estimate exposure of consumers to substances migrating from food packaging materials with important efforts savings. Traditional approaches are based in collecting concentration data directly from the food. The benefit of using these simulation tools is to avoid the analytical difficulties inherent to chemical analysis of food matrices. Data of initial concentration in the packaging materials are still required but these are easier to obtain either through expert judgement or even by analytical means that, depending on the migrant, are typically simpler than those required to analyse food samples. In the present exercise, the use of mathematical simulation combining experimental data and data from an existing database on packaging usage in Portuguese households, allowed to estimate exposure of consumers to BZP present in paper and board food packages, indicating no reason for health concern.

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