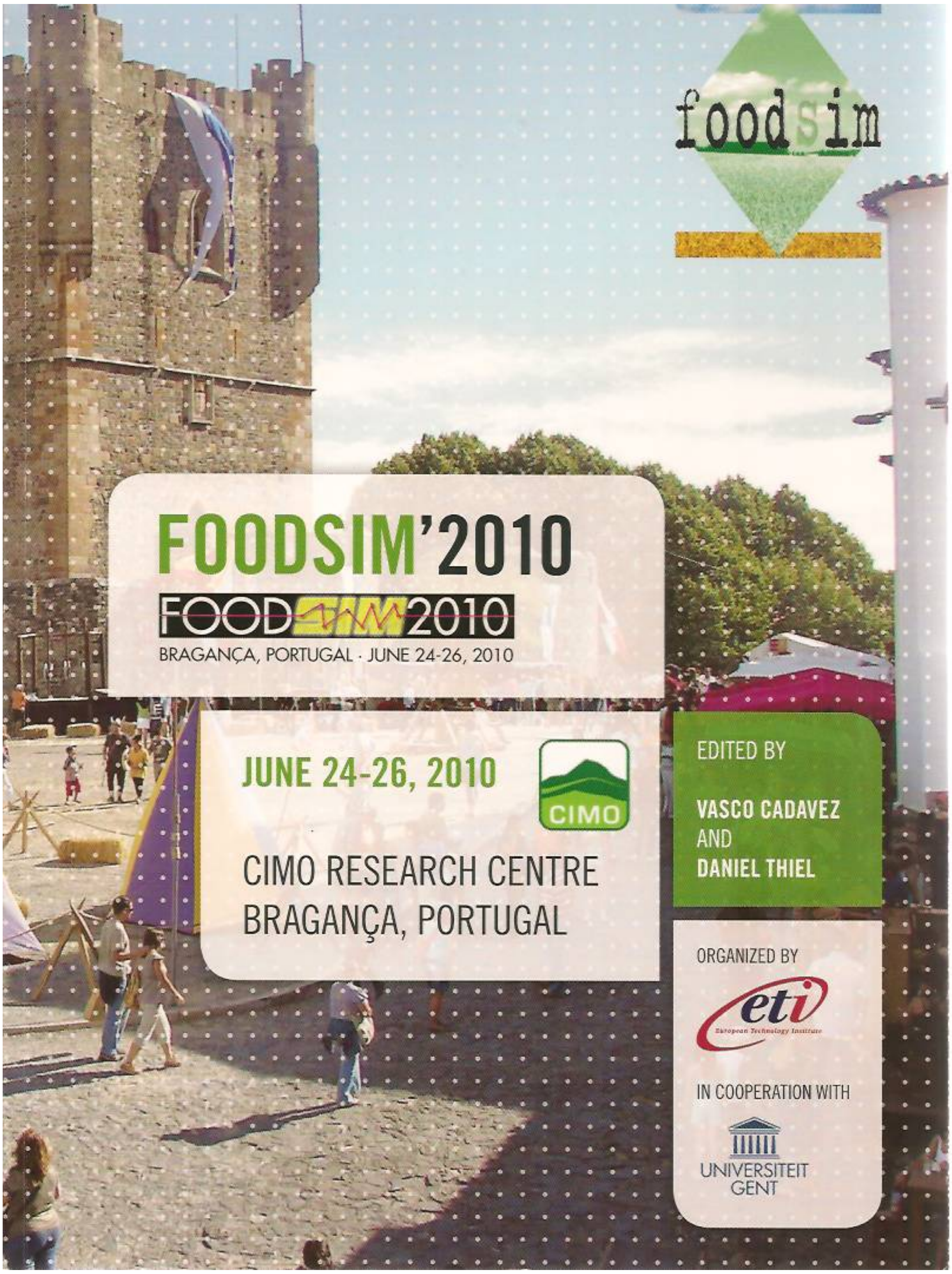
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CONTENTS

PROBABILISTIC SIMULATION OF CHILDREN EXPOSURE TO MIGRANTS FROM PACKAGING: PHOTOINITIATORS FROM PRINTING INKS

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KEYWORDS
Exposure model, benzophenone, packages, food consumption.

ABSTRACT

This paper presents an exercise to simulate exposure of Portuguese consumers to benzophenone, a photoinitiator used in packaging printing inks. The simulation model combines experimental data of benzophenone concentration actually found in packages collected from the market and food consumption and packaging usage data obtained from a database. The model follows a probabilistic approach: the distribution of occurrence data was combines with food consumption data in a probabilistic simulation with the Monte Carlo sampling method. Exposure values found indicate that benzophenone levels of exposure are of no concern healthwise 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 especially for refined assessments, for example exposure assessments of contaminants migrating from food packages (Poças and Hogg 2007). 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 (Peterson 2000).

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 has recently been re-evaluated (EFSA 2009). Although ink is applied in the outer or in an intermediate layer of the packaging material, these ink components can migrate into 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 $_{\text{body weight}}$ (EFSA 2009).

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 which originate 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.

MATERIALS AND METHODS

Exposure model

Exposure of consumer to substances with their origin in packaging systems can be expressed as (Poças and Hogg 2007):

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

Where the *Migration* term represents the concentration of substance that, by transfer from the package, ends in the food; and the term *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.

In this study the concentration on the food was assumed to be the concentration that 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:

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

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

Concentration of BZP in the packages

A short survey of the local market was conducted: samples of paper and paperboard packages were collected and taken to the laboratory for screening analyses. Foods (30) consumed by children and presented in paper and board packaging systems were purchased in one supermarket in Gaia, Portugal, in 2009 and 2010. Food products were mostly dried food such as cookies and biscuits, flour and sugar, cereals and dry pasta, chocolate and butter. The foods all had primary or secondary packages made of paper, paperboard or corrugated board and in some cases there was also an inner package in paper or in a different material and only a few products were in direct contact with the outer packaging.

The packaging materials (only the cellulose based) were extracted with acetonitrile spiked with internal standard at a concentration of 0.5 mg/L, at 70°C for 1 day or 40°C for 2 days. Fifty cm^2 of packaging material was cut into small pieces and extracted with 20 ml of acetonitrile. The extracts were analysed by GC-MS with an external calibration curve fitted by linear regression to data from 5 calibration standards analysed (BZP signal area/internal standard signal area versus BZP concentration). The data was used to generate the probability distribution function to be used of the C_{Pack} term in equation 3.

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

The database from the MIGRAMODEL project (ESB 2008) 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. Results from 628 packaging items were used to generate the probability distribution function of the W_{Pack}/W_{Food} term in equation 3.

Food consumption

The database from MIGRAMODEL project (ESB 2008) was used to provide data on the amount of food in contact with paper and paperboard packages; this database includes data collected at household level. Results from 34 household were used to generate the probability distribution function of the FW term in equation 3.

Probabilistic analysis

The Crystal Ball 7.2.2. (Decisioneering, Inc.) software was used to fit the exposure model inputs as well as the model output to probability distributions functions by the maximum likelihood method. The distributions were truncated to allow only positive values in the exposure model because there is no physical meaning for negative values of these inputs. The goodness-of-fit was assessed by the Anderson-Darling (A-D) test. MC simulation was used as sampling method with 10 000 iterations. Descriptive statistics were calculated from the exposure estimates generated by the model.

RESULTS AND DISCUSSION

Table 1 presents the descriptive statistics for the concentration of BZP found in the cellulosic packages collected from the market. The highest values (9 mg/Kg) were found in boxes of cookies and cereal.

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 1 also presents the data extracted from the MIGRAMODEL database required as inputs in the exposure model. The ratio of packaging material to food weight (W_{Pack}/W_{Food}) presents an average value of 0.14 ranging from 0.002 uo tp 4.6. The total food weight consumed per day and per consumer body weight averaged 0.017 $Kg_{food}/day.Kg_{bw}$. From this total amount of food, an average of 12% has been packaged in paper and board materials (Poças et al. 2009).

Table 2 presents the results for the distribution functions fitting the input variables for the exposure model.

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

Figure 1 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

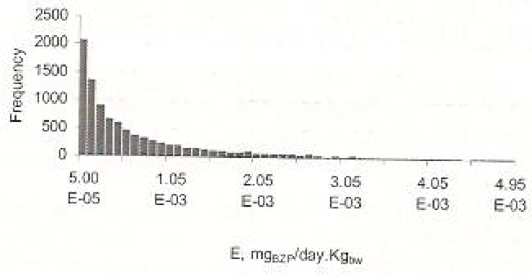

Figure 1. Simulated Exposure to BZP.

Results show mean exposure values 9.97E-4 mg_{BZ}/day.Kg_{bw} and maximum value of 3.1E-2 mg_{BZ}/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 mg_{BZ}/day.Kg_{bw}. These results also indicate that additional efforts in refining the exposure estimates are not required in the present case.

CONCLUSIONS

Simulation models may be applied to estimate exposure of consumers to substances migrating from food packaging materials with important efforts savings (Poças et al. 2010). 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.

Future work will focus on modeling the mass transfer process of components from inks from the secondary package into the food, but considering the barrier of a inner primary package, the time and temperature of storage. That model will be integrated into the exposure probabilistic model.

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