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AN APPROACH TO STOCHASTIC MODELLING OF CONSUMER EXPOSURE FOR ANY SUBSTANCE FROM CANNED FOODS USING SIMULANT MIGRATION DATA

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51 21 Key Words : migration, exposure, threshold, canned foods, metal closures (lids)
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1 Abstract

2 We have constructed a 2 dimensional probabilistic model to estimate the short-term dietary
3 exposure of UK consumers to any generalised migrant from coated light metal food
4 packaging. Using 3 UK National Dietary and Nutrition Surveys (NDNS) comprising 4 - 7
5 day dietary surveys for different age and gender groups, actual body weights and survey
6 years, a sample representative of the dietary consumption of the UK population was obtained,
7 comprising around 4200 food items. Interrogation of the raw data showed that the *per capita*
8 consumption of food and beverage for an adult was 2.9 kg/person/day, being comparable with
9 the USFDA value of 3 kg. The packaging type of each food item was assigned from the
10 survey descriptions or, by sampling from distributions based upon market share information
11 and expert judgement. Each food item was assigned to the relevant food simulant, A
12 (aqueous), B (acidic) or D (fatty) so that simulant migration data could be used. The exposure
13 model was used to evaluate exposure for a given level of migration and, conversely, the level
14 of migration that could be tolerated whilst keeping within a target threshold exposure level.
15 As examples, migration at 10 $\mu\text{g}/\text{dm}^2$ into fatty foods only resulted in an exposure ranging
16 from 0.06 to 0.22 $\mu\text{g}/\text{kg}$ body (actual) weight/day depending on the scenario. The model
17 revealed that if migration from metal coatings was into fatty foods only, migration in the
18 range 1.83 to 4.95 $\mu\text{g}/\text{dm}^2$ (97.5th percentile, depending on the scenario) would give an
19 exposure of less than 1.5 μg per person per day. This is a toxicological threshold limit used in
20 the USA. If migration into simulants A and B is also considered to be at the same level as
21 that for simulant D, then the level of migration for the threshold to be reached is, not
22 surprisingly, lower at (0.64 – 0.87 $\mu\text{g}/\text{dm}^2$) than that if migration were into fatty foods only. In
23 this case, clearly, the main contributors to the exposure were foodstuffs represented by
24 simulants A and B because of their importance in the diet. These estimates are based on 4- or
25 7-days food diaries and chronic exposure over the long term would be expected to be lower.

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For Peer Review Only

1 INTRODUCTION

2 The purpose of this study was to investigate how the extent of consumer exposure to a
3 generalised chemical migrant from food packaging materials may be estimated using
4 migration data obtained with food simulants. We have used a 2-dimensional probabilistic
5 Monte Carlo model [Holmes *et al.* 2005] with, as a test case, the migration of an arbitrary
6 substance from coated light metal packaging. 'Light metal packaging' encompasses food
7 cans, aerosols, tubes and closures such as lids and tops. Single-point estimates and
8 deterministic estimates of exposure to selected migrants from can coatings have been made by
9 others, e.g. for bisphenol A diglycidyl ether [SCF, 2002a] and for bisphenol A [SCF 2002b],
10 but this is the first application of probabilistic modelling. We have tackled this question in
11 two ways. In the first, the exposure that would result from a given level of migration into a
12 food simulant is estimated. In the second approach, using the procedure in reverse, the
13 maximum migration that could be tolerated in order to keep consumer exposure below a pre-
14 defined threshold is calculated.

15
16 The normal approach used by the EU Commission for assessing potential exposure to
17 migrants from packaging, takes a default assumption that an average 60kg individual
18 consumes 1 kg of packaged food each day, that this packaged food is always packed in the
19 material of interest, that the packaging material always contains the substance under
20 consideration, and that the substance is always released from the packaging into the food at
21 the maximum migration limit for that substance [Barlow 1994; CEU 2004]. This exposure
22 model is generally conservative, in that it overestimates exposure in most cases. The default
23 assumptions are used not because they are thought to be realistic, but because in the absence
24 of any other information, this exposure model is generally accepted to be a worst-case for
25 most packaging applications.

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6 2 Previously, a joint industry group for light metal packaging used a per capita approach
7
8 3 [Dionisi *et al.* 2002] to estimate exposure to migrants from canned foodstuffs. Their
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10 4 calculations used statistics for: i) the number of cans manufactured in Europe per year, ii) the
11
12 5 different food types that these cans were used for, iii) the corresponding surface area for each
13
14 6 type of foodstuff, iv) corrections for imports and exports, and v) typical migration levels into
15
16 7 foods. It is clear that that such a *per capita* approach will under-estimate exposure, because a
17
18 8 simple averaging procedure is used and no distinction is made between high, low and non-
19
20 9 consumers of canned foodstuffs. The present study represents a refinement of exposure
21
22 10 estimates, now using actual food consumption statistics and better estimates of packaging
23
24 11 usage. We have used UK food consumption statistics to illustrate this approach. One future
25
26 12 task would be to use statistics for other countries, to see first how easily the statistics could be
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28 13 harnessed in this way and, second, how the estimates compare for different countries.
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36 15 A sample representative of the UK population was obtained using the detailed food
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38 16 consumption records of three UK National Dietary and Nutrition Surveys (NDNS) [UKDA,
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40 17 1990; 1998; 2000]. The surveys provide only limited information on the packaging materials
41
42 18 used for each of the food items. To address this information gap, market share (with
43
44 19 uncertainty) information on food/package combinations were used here. In the following
45
46 20 sections we provide a model overview, describe the data inputs, the process of associating
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48 21 specified food items with the migration concentration data used, and finally the results
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51 22 obtained.
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1 MODEL OVERVIEW

2 A detailed description of the stochastic model used has been published [Holmes *et al.*, 2005].

3 In outline, the daily dose (*DD*) expressed in $\mu\text{g}/\text{kg}$ bw/day is calculated using equation 1.

$$4 \quad DD_{ijk} = \frac{1}{W_j} \sum_{l=1}^{n(k)} w_{ijkl} c_{ijkl} \quad \text{Equation 1}$$

5 Here, DD_{ijk} is the daily dose during iteration i of the model, for individual j on day k
6 consuming up to $n(k)$ items on that day. W_j is the weight of individual j and c_{ijkl} is the
7 concentration of the migrant in the food commodity l whose weight is w_{ijkl} . Depending on
8 the survey duration we calculate the average daily dose for each individual j . For each
9 iteration i uncertain parameter values for the descriptive distributions are sampled, these are
10 then fixed during the subsequent calculations of the exposure for each individual. Exposure
11 across individuals (within an iteration) will vary due to consumption, packaging type and
12 concentration within the food. Exposure for a specific individual (across iterations) will vary
13 due to the packaging type and concentration within the food.

14
15 For this test case therefore, the main tasks were to decide which of the food items in the diary
16 records were packaged in coated light metal packaging, what the consumption of these food
17 items was, and what was the migration concentration data for these food items, leading to a
18 distribution of exposure estimates.

1 DATA INPUTS

3 Food consumption data

4 In each of the NDNS surveys (Table 1) the food consumption of about 2000 individuals is
5 recorded for a 4- or 7-day period. Approximately 4200 individual food item descriptions are
6 used in the surveys.

7 {insert Table 1 about here}

8 *Food item hierarchy.*

9 For this work the NDNS food code list was re-organised into 21 main food group headings
10 such as Bread, Carcass meat and Milk. Each group was then further subdivided, e.g. White
11 bread, Wholemeal bread etc, giving 114 sub-groups. During this stage the food codes were
12 checked to ensure they had been correctly assigned in the NDNS structure. Additionally,
13 where duplicate descriptions occurred we ensured that they were categorised in the same
14 group-subgroups. At the most detailed level there are individual food item descriptions, in
15 some cases with indications of the packaging type. For example, food item 'sweetcorn,
16 canned, drained'. In the 3 surveys there were 884,272 food items consumed in total, covered
17 by about 11,000 different items descriptions when recipe descriptors were included.

19 *Composite foods and Recipes*

20 Some food item descriptions indicated that they are a combination of individual food types,
21 e.g. pre-prepared meal or, due to the preparation or processing, are a combination of food
22 types, e.g. 'Tuna and pasta bake with canned tomatoes and olives'. Clearly, in order to
23 estimate exposure the contributions from the differently-packaged components must be
24 included. To address this issue the NDNS food item codes are identified as whole foods or
25 recipes. Many of the recipes are described in the Risk Recipe Database (RRAD - unpublished

1 FSA internal communication) which break-down the recipe into its ingredient and the
2 proportions in which they occur. For recipes not found in the RRAD a conservative estimate
3 was made of the proportions of each ingredient and the extrapolation factor (see later) was
4 used to account for this. The total number of food items with discrete descriptions consumed
5 in the surveys, following recipe deconstruction etc., was reduced to ca. 4,200.

7 *Observations from raw survey data*

8 The raw data in the NDNS surveys was interrogated to determine what could be understood
9 about the consumption habits of the UK public with regard to consumption of canned food
10 and beverages. This was independent of any stochastic modelling of consumption and
11 potential exposure to migrants. The average daily consumption of food and beverage
12 independent of packaging was calculated for each of the 3 age groups. For adults it was 2.9 kg
13 of food and beverage per person per day, very similar to the value of 3 kg used by the USFDA
14 [CHEESEMAN et al., 1999; Munro *et al.* 2002]. Seniors (>65 years) consumed 2.25 kg
15 whilst Youths (4 to 18 years) consumed 1.7 kg/person/day. The average number of different
16 items of food and beverage consumed daily was 25 for youths, 36 for adults to 39 items per
17 person per day for seniors. The eating habits of the three age groups are different. It should
18 also be noted that dietary habits may, and probably will, have changed since the surveys were
19 conducted.

20
21 To determine the level of consumption of canned food and beverages, all items that were
22 described as canned or were almost certainly canned (e.g. corned beef) were placed into 3
23 groups. These were canned beverages, canned foods and canned foods that formed part of a
24 meal. Only 17 out of 2197 (0.8%) of adults did not consume a canned item (food or
25 beverage) during the survey period. Similarly, only 92 out of 1687 (5.5%) Seniors and 6 out

1 of 1701 (0.4%) youths did not consume canned items during the survey periods. The average
2 weight of food and beverage, explicitly recorded in the surveys as being canned, consumed by
3 seniors was 0.13 kg/person/day, 0.18 kg for adults and 0.17 kg for youths. This was for actual
4 consumers (non-consumers were not included). Table 2 shows the weight of canned food
5 consumed daily. These figures are undoubtedly too low because, as discussed elsewhere
6 [ILSI, 1997; Holmes et al., 2005] past food surveys have not recorded packaging usage well,
7 if at all, because the surveys were not conducted with this application in mind. Consequently,
8 packaging usage has to be estimated separately (see later)

9
10 {insert Table 2 about here}

1 Migrant concentration data

2 All relevant food items that are identified and consumed within the dietary surveys must be
3 associated to their migration data. Food simulants are used to test for the general case, for
4 contact with a variety of foods of the same or similar class, and so in this treatment for any
5 generic migrant we have set up the model to use food simulant migration data. There are no
6 food simulants explicitly listed in EU regulations for testing polymeric coatings on light metal
7 packaging, but for plastics the simulants listed in Table 3 are specified according to the type
8 of food that is intended to be packed [CEU 2002; 2003].

9 {insert Table 3 about here}

10 Migration data for simulants are generally reported on a surface area basis in units of $\mu\text{g}/\text{dm}^2$.
11 In this study we consider an arbitrary migrant with a migration level of either 0 or $10 \mu\text{g}/\text{dm}^2$
12 into the aqueous simulants A and B (distilled water for aqueous foods; 3% acetic acid for
13 acidic foods) and for simulant D (fatty foods). Beverages were excluded from this evaluation,
14 as their can coatings tend to be specific to beverages. Since this study is restricted to foods
15 and not beverages the simulant C (10% ethanol solution, for alcoholic beverages) is not
16 considered. The Plastics Directive [CEU 2002; 2003] allows for a correction of simulant D
17 migration data by a reduction factor to account for the aggressive character of simulant D
18 (olive oil) compared to most fatty foods. However, for can coatings where the food is
19 retorted, it can be argued that these reduction factors are questionable because the severe heat
20 processing conditions that the thin polymeric coating experiences, can give rise to exhaustive
21 migration even with low-fat foods. So the model was run both using and then not using these
22 reduction factors, which are in the range 2-5. In the model, the corresponding simulant and a
23 reduction factor if applicable, was assigned to every item of foodstuff recorded in the surveys.

24

1 **Conversion factors**

2 When migration levels are expressed per unit surface area (i.e. $\mu\text{g}/\text{dm}^2$) the EU standard

3 conversion to a mass basis is achieved by a multiplication with the factor $6\text{dm}^2/\text{kg}$, for a

4 standard 10 by 10 by 10cm packaging cube of a food with density of 1. However, it is

5 apparent that the actual packaging types can cover a range of contact scenarios where this 6:1

6 ratio is inappropriate. Improved conversion factors (CF) for the surface area/mass ratios were

7 calculated using the actual ranges encountered for the different can sizes.

8 Can sizes (contents mass and surface area) with their market shares by country [Dionisi *et al.*

9 2002] were averaged for each food type (including beverages). Three size ranges were

10 established which encompassed all of the food types and these are shown in Table 4. The

11 food types of fruit, vegetables, soups, dairy produce, ready meals and other foods all had a

12 similar range and were defined as ‘Regular’. Meat and fish had distinctly higher ranges.

13 The can sizes for beverages may range from 150ml – 500ml with respective surface areas of

14 $1.8 - 4.1 \text{ dm}^2$. These values gave a conversion factor in the range 8 to $12 \text{ dm}^2/\text{kg}$, thus

15 beverage cans were assigned ‘Regular’ conversion factors.

16 For closures (i.e. lids on bottles and jars), two main sizes were allocated (small and large)

17 with conversion factors representing the ranges typically found. This reflects the significantly

18 smaller surface areas found when mixed packaging is considered. Similarly, conversion

19 factors for tubes and aerosols were also be calculated. The values used are given in Table 4.

20 {insert Table 4 about here}

21 **Extrapolation factors**

22 In some cases the concentration data do not correspond directly to the food item description.

23 As an example consider the food item ‘*corned beef hash*’. Assuming that the corned beef was

24 canned (i.e. 100% market share), if a dietary record showed that a person consumed 100g of

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3 1 corned beef hash, it is clear that they did not consume 100g of canned corned beef. In this
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5 2 case, and in the absence of recipe information from the RRAD (see above) it was estimated
6
7 3 that the amount of corned beef in the recipe was 50%, ranging from 30% to 70%. To allow
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9 4 for this, an extrapolation factor (EF), defined as a triangular distribution with range [0.3, 0.5,
10
11 5 0.7] was used to correct the total recipe weight to a mass of canned corned beef consumed.
12
13 6

7 **Market share**

8 In order to calculate the dose due to the migrant in a particular food item we must establish
9 the packaging type. In the case of canned foodstuffs, often the NDNS food item descriptions
10 enable the packaging type to be identified directly, i.e. are definitely packaged in metal e.g.
11 '*Custard, low fat canned*'. For these items the market share is 100%. For those items
12 definitely not packaged in coated metal, then the market share is 0%. Example '*salmon, raw*'
13 or '*grape juice carbonated not canned*' and so these items do not contribute toward the
14 exposure.
15

16 For the remaining food items, whilst the market shares of different packaging types are
17 known at a manufacturing level, in most cases detailed information at the level of each
18 individual food item is not available. For these cases it is necessary, using expert judgement,
19 to estimate the market shares (with uncertainty) of the packaging(s) of interest, e.g. 20±20%
20 can, 25±20% large closure, 25±20% small closure and 30±20% other. This information
21 would then be sampled from a triangular distribution with range [0, 0.2, 0.4] etc.
22

23 **Packaging Loyalty**

24 Packaging loyalty is indicated if the individual's consumption of a given package type is
25 greater than would be expected from market share. Consumers who exhibit loyalty will have

1 higher exposure. To explore the importance of packaging loyalty we adopted two options,
2 zero package loyalty and total package loyalty. Zero package loyalty, as it's name suggests,
3 indicates that a consumer will choose an item with a specific package type with proportions
4 equal to the market shares of the package types, i.e. shows no bias toward any one package
5 type. In contrast, total package loyalty is where an individual will always choose an item with
6 the same package type. For example, they will always tend to choose a particular food
7 product in a metal can in preference to a plastic pouch or a glass jar, or *vice versa*. Clearly,
8 packaging loyalty is linked to brand loyalty. To implement package loyalty, we applied it at
9 the food group level and fixed the package type of the food items contained within that group
10 to that of a random sample from the package types using the market share values. This is a
11 simplification that removes the need to apply loyalty to each food item consumed. In fact this
12 has an added advantage because even if packaging loyalty was applied to each item, it would
13 be expected that to some extent the same packaging loyalty would operate across similar food
14 items.

1 COMBINING THE FOOD CONSUMPTION AND PACKAGING DATA WITH THE 2 SIMULANT MIGRATION DATA

4 **Grouping similar food items**

6 To manage the large number of individual food items, they were gathered together into
7 groups for which the same parameters applied; regarding packaging type, concentration data,
8 conversion factor, extrapolation factor, market share, etc. It is possible to group at a high
9 (coarse) level, with many items in a few groups, or at a low (detailed) level with a few items
10 in many groups. The lowest level grouping required inspection and grouping of 4,200
11 individual items. The approach used was to select those items which were definitely canned
12 (100% market share) and those which were definitely not canned (0% market share). Expert
13 judgement was used to allocate a market share for the remainder. The items which were, or
14 could possibly be, canned were then further sub-divided and grouped. This grouping was at
15 various levels and in some cases was according to type of foodstuff (simulants), type of
16 container (can, closure, aerosol, tube), size of can (fish or regular, for example) or closure,
17 part or whole of meal as outlined earlier.

19 The different groups which form the basis for the models are given in Tables 5 and 6, where it
20 can be seen that the low level (detailed) grouping consisted of 66 groups compared to 4
21 groups for the high level (coarse) groupings. The more refined the segregation into groups
22 the more realistic the assumptions, because specific and different factors can be applied to
23 each group. Runs denoted by T1, T2 or T3 were based on the high level grouping, whilst the
24 others (T4, T4 and T5) used the low level grouping.

{insert Tables 5 and 6 about here}

For the low level groupings, items were identified which could be in a can or jar. For example, sauces could be in a can (high surface area) or jar (relatively low surface area of lid). A conservative assumption of 50% market share (with an associated uncertainty distribution) for sauces being in a can was made, with jars having the remaining market share. For this case it was assumed that none were packaged in plastic. Table 7 illustrates how data were associated for a foodstuff, which could be in a jar or can. In other cases it was possible that some of the food could be packaged in alternative forms of packaging, such as retort plastic. A market share representing a conservative case (highest usage) for metal packaging, with an associated range, was allocated. In Table 7, the group contains foods represented by simulant D/4 packaged in either cans or jars. The conversion factors of [7, 11, 19] represent the surface area to weight range for meat cans and [0.35, 1.2, 4.0] represents that for large closures (lids). Each package type was assigned a $50\% \pm 25\%$ market share. The extrapolation factor is 0.25 because the foodstuff is simulant D/4 and the simulant D reduction factor was applied for this particular run. If it were not then the extrapolation factor would be 1.

{insert Table 7 about here}

Combining concentration data with groups

For the general case, migration of a substance into different simulants from light metal packaging can be used to estimate exposure to that substance using the CSL stochastic model [Holmes et al., 2005]. Various scenarios about a migrant into foodstuffs were used in order to compare their impact on the exposure. These scenarios covered the nature of the migrant (e.g. only fat-soluble, only water-soluble etc) and the availability of migration data on a concentration- or area-related basis.

1. A species migrated into fatty foodstuffs (simulant D) only and that migration into foodstuffs represented by simulants A, B and C was a true zero[†]

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5 2 2. The simulant D reduction factor was or was not applicable
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9 4 3. Migration was either at $10\mu\text{g}/\text{dm}^2$ or $60\mu\text{g}/\text{kg}$
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11 5

12 6 4. Migration into simulant D foods, which are in cans only, with migration into A, B and C
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14 7 being a true zero[†].
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16 8

17 9 5. Migration into simulant A or B foods, which are in cans only, with migration into D
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19 10 being a true zero[†].
20
21 11

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23 12 6. Migration into simulant A or B or D foods, which are in cans only.
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25 13

26 14 [†] either because migration does not occur into that food/ simulant type or, more fundamentally,
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28 15 because different coating chemistries are used for different food types, which do not contain a
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30 16 residue of the substance.
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33 18 The "definitely not canned" group, vitamins etc, as well as beverages were not associated with
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35 19 any concentration data and were therefore not used in any of these evaluations. Beverages
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37 20 were excluded from this evaluation, as their can coatings tend to be specific to beverages.
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1 RESULTS AND DISCUSSION

3 Models run

5 Eight runs of the model were used to represent the above scenarios.

7 T1 to T5 considered migration only into simulant D foodstuffs packaged into cans, jars, tubes
8 and aerosols. Furthermore, the migration was at a single fixed value thus variation between
9 level of detection and the fixed value was not used. Migration into A, B, C was a true zero,
10 thus they did not contribute to exposure from the groups assigned to simulants A, B, C or O.
11 However, if two simulants are representative for a particular foodstuff, such as (B, D/3) (a
12 food both acidic and fatty) then that item was allocated the D concentration data. The
13 differences in T1 to T5 are:

15 T1 (high level) assumed that the simulant D reduction factor was not applicable and migration
16 was at 60 µg/kg.

18 T2 (high level) assumed that the simulant D reduction factor was not applicable and migration
19 was at 10 µg/dm². In addition a conversion factor to represent the different sized containers
20 was applied and due to the coarse grouping, a wide range was used [0.08, 6, 19] dm²/kg.

22 T3 used the same assumptions as T2 but the simulant D reduction factor was applied.

24 T4 (low level) assumed that the simulant D reduction factor was not applicable and migration
25 was at 10µg/dm². Conversion factors appropriate for the different sized packages were
26 applied.

28 T5 (low level) assumed that the simulant D reduction factor was not applicable and migration
29 was at 60 µg/kg.

31 T4-D, T4-AB, T4-ABD (all low level) were models for canned foods only (aerosols, tubes
32 and closures were excluded) and assumed that the same coating would be used for all the
33 canned food items. It was assumed that the substance only migrated into D foods (T4-D) with

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3 1 A and B foods being a true zero or *vice versa* (T4-AB) or the substance migrated equally into
4 all foods (T4-ABD). In those instances where a food item could be allocated more than one
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6 2 all foods (T4-ABD). In those instances where a food item could be allocated more than one
7
8 3 simulant, such as (B, D/3), then depending on the above scenario the migration was allocated
9
10 4 either that for B or D. In both these cases, the actual value was the same, thus that food item's
11
12 5 contribution to exposure was the same since the simulant D reduction factor was not used in
13
14 6 these runs. Migration was a single fixed value of 10 $\mu\text{g}/\text{dm}^2$.

7 8 **Exposure**

9
10 The results from the above eight models run for the 97.5 percentile consumer for each age
11
12 11 group are shown in Table 8. The data are in μg per kilo body weight (actual) per day - $\mu\text{g}/\text{kg}$
13
14 12 bw/day - or $\mu\text{g}/\text{person}/\text{day}$ and are for the three age groups, youths, adults and seniors.

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27 14 {Insert Table 8 about here}

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30 16 Considering models T1 to T5, initially, the following can be concluded.

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34 18
- 35 • The use of a simulant D reduction factor reduces the exposure by a factor slightly
36 greater than 2 (T2 cf T3) from (0.1 – 0.22) to (0.05 – 0.09) $\mu\text{g}/\text{kg}$ bw/day.
37
38 20
 - 39 • Refining the groupings (T2 cf T4 and T1 cf T5) reduces the exposure, but only slightly
40 from (0.1 – 0.22) to (0.11 – 0.17) and (0.07 – 0.16) to (0.06 – 0.1) $\mu\text{g}/\text{kg}$ bw/day.
41
42 22
 - 43 • Using $\mu\text{g}/\text{dm}^2$ instead of $\mu\text{g}/\text{kg}$ of food increases the exposure (T1 cf T2) (0.07 – 0.16)
44 to (0.1 – 0.22) (T4 cf T5) (0.11 – 0.17) to (0.07 – 0.1) $\mu\text{g}/\text{kg}$ bw/day.
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46 24
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50 27 Figure 1 displays these results in units of $\mu\text{g}/\text{kg}\text{-bw}/\text{day}$ for the 97.5th percentile consumer,
51
52 28 together with the 95th – percent (2 standard deviations) confidence range on the uncertainty
53
54 29 associated with the inputs.

55
56 30
57 31 {insert figure 1 about here}

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2
3 1 Model T1 shows the exposure assessment assuming a $60\mu\text{g}/\text{kg}$ migration into simulant D and
4 has selected food items only appropriate to that simulant based on the Food group/subgroup
5 descriptions. The only source of uncertainty in this model is from the market share values.
6
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9 4 Exposure in this model is dependent upon the individual's consumption of the affected items.
10
11 5 As can be seen in the Table 7 and Figure 1, the model T2 produces the highest exposure
12 assessment across all of the surveys with the greatest uncertainty due to the conservative
13 uncertainty range imposed on the conversion factors. T3 indicates a proportionate reduction
14 7 by the introduction of the simulant D/X reduction factors. Model T4 illustrates that
15
16 8 examining individual food items and associating more appropriate conversion/extrapolation
17 9 factors to the refined groups, has the effect of reducing the exposure estimates and reducing
18
19 10 the associated confidence range of the estimate. Model T5 is equivalent to model T1 but uses
20
21 11 the refined baskets. This indicates how an exposure estimate is reduced by applying more
22
23 12 accurate associations to the concentration data.
24
25 13
26 14

27 28 15 *Contributors to exposure*

29
30 16 To explore what factors are involved within these models, additional analysis is required. An
31 obvious property to investigate is the percentage contribution of each of the food baskets, for
32 17 example for the model T2 this is shown in Figure 2. As can be seen, the primary contribution
33 18 of the exposure comes from the basket for items assigned simulant B, D which contained
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35 19 canned vegetables i.e. highest consumed items.
36
37 20
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40 22 {Insert Figure 2 about here}
41
42 23

43
44 24 Considering Table 8, it can be seen that the main contributors to exposure from canned foods
45 25 are those represented by simulants A or B (T4-AB). This is about 3 times greater than those
46 26 foodstuffs represented by simulant D (T4-D) $0.26 - 0.52$ cf $0.11 - 0.17 \mu\text{g}/\text{kg bw}/\text{day}$. It is
47
48 27 not surprising when one considers the types of food and their consumption. The results for
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50 28 migration into A, B plus D (T4-ABD) does not equal the sum from the other two models, due
51
52 29 to the fact that some foods consumed were allocated mixed simulants, such as B, D/3 and they
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54 30 would have contributed to exposure in both models T4-AB and T4-D.
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Derivation of a threshold migration level

Coated metal packaging, like other forms of packaging, may give rise to a number of migrants at low levels that are neither starting substances (monomers) or additives [ILSI, 2002]. It is practically impossible to identify, isolate or synthesise, and assess the hazard of each and every one using conventional toxicity tests. This situation is not unique to packaging migrants and a generalised approach to deal with the issue has been proposed. The threshold of toxicological concern (TTC) is a principle which refers to the establishment of a generic human exposure threshold value for chemicals below which there would be no appreciable risk to human health. [ILSI, 2000; KROES *et al.*, 2004; Barlow, 2005]. For chemical migrants from food contact materials, the US-FDA uses a threshold exposure of 1.5 ug per person per day [MUNRO *et al.*, 2002] and we shall use this value for the purpose of illustration here.

It is possible from the exposure resulting from migration at 10 $\mu\text{g}/\text{dm}^2$ to estimate the level of migration corresponding to an exposure ceiling of 1.5 $\mu\text{g}/\text{person}/\text{day}$ for the 97.5%-ile for the scenarios represented above, as shown in Table 9. It should be borne in mind that this assumes that the only source to exposure of the substance is from canned fatty foods.

{insert Table 9 about here}

Without simulant D reduction factors, an exposure of 1.5 $\mu\text{g}/\text{person}/\text{day}$ equates to a migration limit of 1.83 to 2.61 $\mu\text{g}/\text{dm}^2$ (T2 and T4).

With the use of simulant D reduction factors this is increased to 4.02 to 4.95 $\mu\text{g}/\text{dm}^2$.

Migration at 15 to 19 $\mu\text{g}/\text{kg}$ (T1) or 22 to 28 $\mu\text{g}/\text{kg}$ (T2) corresponds to an exposure of 1.5 $\mu\text{g}/\text{person}/\text{day}$.

Not unexpectedly if a substance migrates at 10 $\mu\text{g}/\text{dm}^2$ into all foods represented by simulants A, B and D, or A and B then the migration threshold is low being $< 1 \mu\text{g}/\text{dm}^2$. However, if migration occurs only into those foodstuffs represented by simulant D, then a threshold of about 2 $\mu\text{g}/\text{dm}^2$ is possible. Note that this is for the actual surface areas encountered and not

1 the traditional 6dm²/kg used by the EU. The range used was from 6 to 19 dm²/kg (Table 4).
2 This threshold level of migration is still a conservative estimate due to the fact that different
3 coatings are used for different foodstuffs and the species migrating from one could be
4 different to those from another. In order that a more refined estimate for a migration
5 corresponding to a threshold is obtained it would be possible to consider the individual
6 coatings and their likely migrants into different foods on a case by case basis. It should also
7 be recognised that these estimates for the 97.5th percentile consumer are based on 4- or 7-day
8 food diary records and chronic exposure would be expected to be lower over longer periods of
9 time.

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For Peer Review Only

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24 10 conclusions in this paper are the responsibility of the authors alone and they should not be
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27 11 taken to represent the opinion of the sponsors of this work.
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1 **Table 1.** Summary of the NDNS surveys used in this paper.

Year	Group	Duration	Number of people	Reference
1986/7	Adult 16 – 64 years	7 days	2197	UKDA, 1990
1994/5	Senior over 65 years	4 days	1733	UKDA, 1998
1997	Youth 4 – 18 years	7 days	1701	UKDA, 2000

2
3 **Table 2.** Daily consumption of explicitly-coded canned foods and beverages for the 3 age
4 groups (consumers only)
5

Daily consumption (kg/day)	97.5th %-tile	2.5th %-tile	50th %-tile
Youth food	0.518	0.016	0.126
Youth beverage	0.090	0.001	0.019
Adult food	0.466	0.024	0.135
Adult beverage	0.128	0.001	0.024
Senior food	0.306	0.009	0.095
Senior beverage	0.160	0.001	0.029

6
7 **Table 3.** Food simulants specified for testing plastics for migration (CEU 2002, CEU 2003)

Simulant code	Composition of the simulant	Foodstuffs that the simulant represents
A	Water	aqueous foods with a pH > 4.5
B	3% w/v Acetic acid	Acidic foods pH ≤ 4.5
C	10% v/v Ethanol	Alcoholic foods & beverages
D (D/X *)	Olive oil or alternative fat simulants	Fatty foods * Test value divided by reduction factor X, in the range 2 to 5, because olive oil is too severe for less fatty foods
O	No testing required	For example fruits with a peel

1 **Table 4.** Surface area to weight (dm²/kg) ratios for different types of cans and packaging for
 2 food.
 3

	Lowest	Median	Highest
Can use			
Regular (R)	6	8	12
Meat (M)	7	11	19
Fish (F)	14	17	19
Closure Type			
Small (S)	0.08	0.2	0.8
Large (L)	0.35	1.2	4.0
Tubes	10	13	16
Aerosols	12	14	16

1 Table 5. Low level (detailed) groups definitions used in model T4 and T5.

Group Description	No. of items	Group Description	No. of items
100% not canned	3167	Can R/closure L (50/50) 100% M/S sim D/5	5
Small closure 75% M/S sim O	1	Can R/closure L (50/50) 100% M/S sim B	5
Small closure 75% M/S sim D/3	15	Can+can/closure in meal 100%M/S EF0.5 sim B	8
Small closure 75% M/S sim B	12	Can tom 100% M/S EF 0.2 sim B	6
Small closure 75% M/S sim A	14	Can R/closure L (50/50) 50% M/S sim D/4	1
Sauce closure 100% M/S sim O	1	Can R /closure L (50/50) 100% part meal sim B	22
Possibly can M 30% M/S sim D/5	55	Can meat meal 100% M/S EF 0.5 sim D/4	10
Possibly can M 30% M/S sim A, D/4	3	100% canned items sim D/5	7
Possibly can 50% M/S sim D/5	5	100% canned items sim D/4	19
Possibly can 50% M/S sim D/4	4	100% canned items sim D/3	7
Possibly can 50% M/S sim D/2	2	100% canned items sim D	9
Possibly can 50% M/S sim B,D/3	1	100% canned items sim C*	9
Possibly can 50% M/S sim B	6	100% canned items sim C	13
Possibly can 50% M/S sim A	28	100% canned items sim B, D/3	9
Possibly can 30% M/S sim O	5	100% canned item sim B	90
Possibly can 30% M/S sim D/4	5	100% canned item sim A, D/4	7
Possibly can 30% M/S sim D/3	2	100% canned item sim A	65
Possibly can 30% M/S sim B, D/5	5	Tubes simulant D/3	1
Possibly can 30% M/S sim B	1	Tubes part of meal Sim B	2
Possibly can 30% M/S sim A	4	Tubes B, 100% MS	6
Large closure 50% M/S sim D/5	1	Tube simulant A	2
Large closure 50% M/S sim D/4	2	Simulant B, part of closure sauce only L	2
Large closure 50% M/S sim D/3	13	Sim B canned 100% part of meal	2
Large closure 50% M/S sim A, D/4	12	Large closure D/5 M/s 50% part of meal	14
Large closure 50% M/S sim A	6	Closure S part of meal 50%MS sim B EF 0.1	2
Large closure 100% sim D/5	1	Closure L Sim B 50% M/S	3
Large closure 100% M/S sim O	1	Can closure 50/50 part of meal simulant B	4
Large closure 100% M/S sim D/3	6	Aerosol D/2 100% M/S	1
Large closure 100% M/S sim D	1	100% canned fish sim D/3	3
Large closure 100% M/S sim B	31	100% canned fish sim B,D/3	6
Large closure 100% M/S sim A	12	100% canned fish sim A	20
CanR/closureL 50% M/S sim B, D/5	1	Vits medicines & toddlers	283
CanR/closureL (50/50) 50% M/S sim A, D/4	1	Beverages	154
		Total items	4221

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3 R-Regular can size, L-Large closure, S-Small closure. All groups use the appropriate conversion
4 factors as defined in Table 4 depending upon the group contents.

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2 **Table 6.** High level (low level of detail) groups used in the minimal knowledge models T1,
3 T2 and T3

Group Description	No. of items
*Extrapolation factor X = 1 for T1, T2 and X = 3 for T3	
Not canned, simulants A, B, C	3498
100% canned, simulant B, D/X*	6
Simulant D, estimated market share as canned 50%	76
Simulant D/X* (meat), estimated market share as canned 5%	641

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6 **Table 7.** Association table for a food group with input data for more than one type of metal
7 packaging.
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Package type	Concentration group	Conversion factor			Extrapolation factor			Market share		
		Min	Best estimate	Max	Min	Best estimate	Max	Min	Best estimate	Max
Can	Simulant D	7.0	11.0	19.0	0.25	0.25	0.25	25.0	50.0	75.0
Closure L	Simulant D	0.35	1.2	4.0	0.25	0.25	0.25	25.0	50.0	75.0
Other	0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0

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Table 8 Exposure to a migrant from coated light metal packaging

Model	Grouping	Simulant concentration data		Surface area/weight ratio range	Simulant D reduction factor	Exposure $\mu\text{g}/\text{kg}$ actual body weight/day			Exposure $\mu\text{g}/\text{person}/\text{day}$		
		D	A, B			Youth	Adult	Senior	Youth	Adult	Senior
T1	Coarse*	60 $\mu\text{g}/\text{kg}$	0	Not used	Not used	0.16	0.08	0.07	5.72	5.55	4.76
T2	Coarse*	10 $\mu\text{g}/\text{dm}^2$	0	0.08, 6, 19	Not used	0.22	0.11	0.10	7.67	7.68	6.78
T3	Coarse*	10 $\mu\text{g}/\text{dm}^2$	0	0.08, 6, 19	D/X	0.09	0.05	0.06	3.03	3.61	3.73
T4	Detailed*	10 $\mu\text{g}/\text{dm}^2$	0	Actual	Not used	0.17	0.11	0.13	5.74	8.09	8.19
T5	Detailed*	10 $\mu\text{g}/\text{dm}^2$	0	Not used	Not used	0.10	0.06	0.07	3.20	4.17	4.04
T4-ABD ⁺	Detailed*	10 $\mu\text{g}/\text{dm}^2$	10 $\mu\text{g}/\text{dm}^2$	Actual	Not used	0.56	0.30	0.35	17.17	20.34	23.42
T4-AB ⁺	Detailed*	0	10 $\mu\text{g}/\text{dm}^2$	Actual	Not used	0.52	0.26	0.32	15.12	17.39	20.64
T4-D ⁺	Detailed*	10 $\mu\text{g}/\text{dm}^2$	0	Actual	Not used	0.17	0.11	0.13	5.66	7.96	8.16
* refer to Tables 5 and 6 for further details											
⁺ food only – excludes closures, aerosols and tubes											

Table 9 Migration from coated light metal packaging which corresponds to an exposure of 1.5 µg/person/day

Model	Grouping	Simulant concentration data		Surface area/weight ratio range	Simulant D reduction factor	Migration µg/dm ²			Migration µg/kg		
		D	A, B			Youth	Adult	Senior	Youth	Adult	Senior
T1	Coarse*	60 µg/kg	0	Not used	Not used				15.75	16.23	18.93
T2	Coarse*	10 µg/dm ²	0	0.08, 6, 19	Not used	1.95	1.95	2.21			
T3	Coarse*	10 µg/dm ²	0	0.08, 6, 19	D/X	4.95	4.16	4.02			
T4	Detailed*	10 µg/dm ²	0	Actual	Not used	2.61	1.85	1.83			
T5	Detailed*	10 µg/dm ²	0	Not used	Not used				28.15	21.56	22.30
T4-ABD ⁺	Detailed*	10 µg/dm ²	10 µg/dm ²	Actual	Not used	0.87	0.74	0.64			
T4-AB ⁺	Detailed*	0	10 µg/dm ²	Actual	Not used	0.99	0.86	0.73			
T4-D ⁺	Detailed*	10 µg/dm ²	0	Actual	Not used	2.65	1.89	1.84			
* refer to Tables 5 and 6 for further details											
+ food only – excludes closures, aerosols and tubes											

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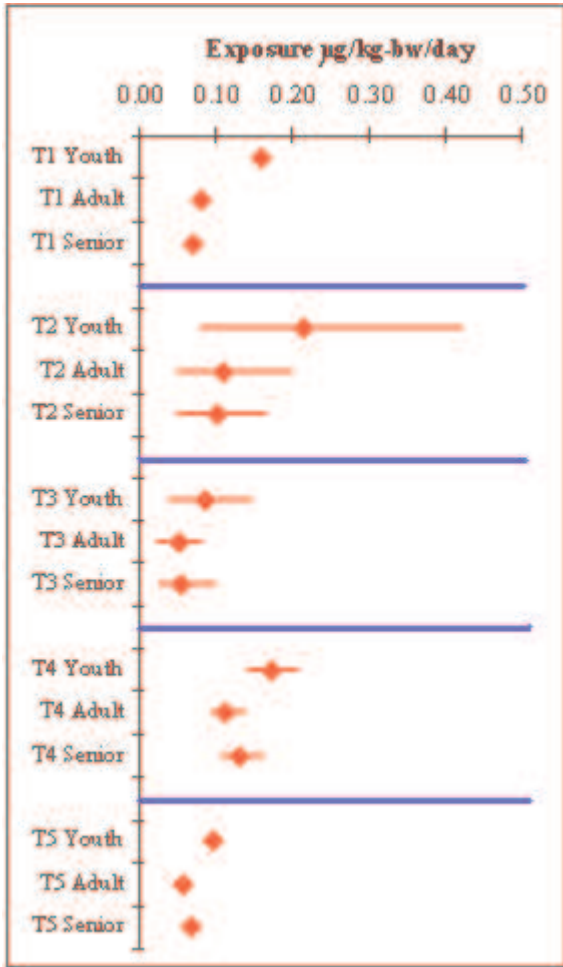


Figure 1. This graph shows the 97.5th – percentiles for the different age groups for the different threshold models run. Red diamonds indicate the median values as shown in Table 8 and the red lines give the 95 percent confidence range for each estimate.

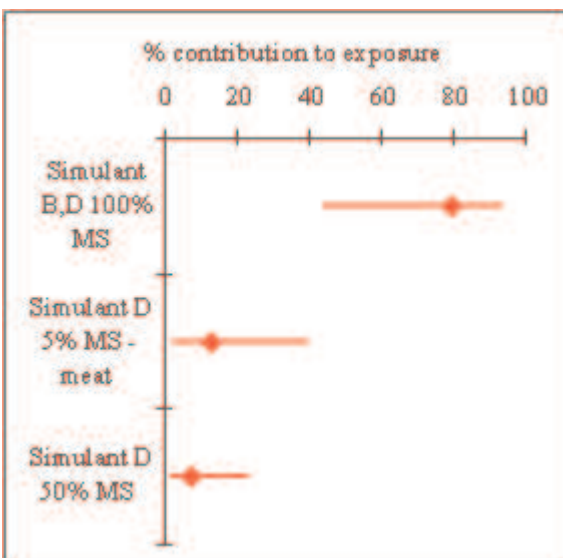


Figure 2. Percentage contribution to the exposure from the food baskets as defined in model T2 for the youth survey. Again diamonds indicate median values and lines denote the 95 percent confidence range.