

JRC TECHNICAL REPORTS



Training workshop "Safety of food contact materials: exposure assessment of chemicals in foods and the use of FACET for exposure assessment"

Ispra, 07 October 2014

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Abstract

Two concurrent Workshops on " Safety of food contact materials: migration testing and exposure assessment of chemicals in foods" are organised by the JRC's European Reference Laboratory for Food Contact Materials on 07-08 October 2014 in Ispra. These workshops were dedicated to training and exchange of information capacity building for National Reference Laboratories, Member States and stakeholders in the area of safety of food contact materials. It also includes a special opportunity for participation under EC's Enlargement & Integration activities.

This report presents the specific workshop on the use of FACET. The Flavourings, Additives, food Contact materials Exposure Tool (FACET) is a novel exposure tool which was created as an FP7 EU funded research project which ran from 2008 to 2012. The JRC, beyond its participation as project partner, was designated as responsible entity for the dissemination and sustainability of the tool. A workshop was offered on the newest exposure tool for the prediction of exposure assessment of chemicals in foods including food contact materials. A demonstration of the tool was dedicated for the first time to NRLs and/or Member States and could include optional participation to other interested stakeholders including opportunity for participation under EC's Enlargement & Integration activities.

Executive Summary

Ensuring that what we eat is safe does not stop at testing the food itself. Everything that comes in contact with food as it is produced, packaged, transported, stored, prepared and consumed also needs to be safe. European legislation on food contact materials has a long history.

Two concurrent Workshops on " Safety of food contact materials: migration testing and exposure assessment of chemicals in foods" were organised by the JRC's European Reference Laboratory for Food Contact Materials on 07-08 October 2014 in Ispra. These workshops were dedicated to training and exchange of information capacity building for National Reference Laboratories, Member States and stakeholders in the area of safety of food contact materials. They also included a special opportunity for participation under EC's Enlargement & Integration activities.

This report presents the specific workshop on the use of FACET. The Flavourings, Additives, food Contact materials Exposure Tool (FACET) is a novel exposure tool which was created as an FP7 EU funded research project which ran from 2008 to 2012. The JRC, beyond its participation as project partner, was designated as responsible entity for the dissemination and sustainability of the tool. A workshop was offered on the newest exposure tool for the prediction of exposure assessment of chemicals in foods including food contact materials. A demonstration of the tool was dedicated for the first time to NRLs and/or Member States and could include optional participation to other interested stakeholders including opportunity for participation under EC's Enlargement & Integration activities.

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Workshop training programme

The programme included:

- Overview of FACET and its capabilities
- Getting started (including hands-on exercises)
- Outputs and reports etc.
- Pre-population (hands on exercises)
- More advanced options
- Users' experiences and lessons learnt/ debriefing
- Discussion and summing up

The specific agenda is presented below. The trainers were S. Kelly and A. Connolly from CremeGlobal who were the modellers in the FP7 project FACET and contribute to the sustainability of the tool together with the JRC.

FACET Food Contact Materials

- Overview of FACET Packaging
 - Basic Packaging Assessment (Example): BPA for UK 19-64 year olds
 - Statistical Terminology and Examples
 - Basic Packaging Assessment (Exercise): Styrene for UK 19-64 year olds
 - Assess Lowest Tiers (Example): BPA for UK 19-64 year olds
 - Assess Lowest Tiers (Exercise): Styrene for UK 19-64 year olds
- Creating your own Concentration Data table and running an exposure assessment
- Exporting Graphs, Data and Reports from FACET
- Discussion and Questions
- Advanced Packaging Features: Creating a New Packaging Structure for a Food and Running an Exposure Assessment for a chosen substance.
- Discussion and Questions

FACET Flavourings

- Overview of FACET Flavourings
 - Basic Flavouring Assessment (Example): Isoamyl Acetate (Fl. No. = 9024)
 - Basic Flavouring Assessment (Exercise): Trans-2-Hexenal (Fl. No. = 5073)
- Refined Flavouring Assessment using Probability of Addition (Example): Isoamyl Acetate
- Discussion and Questions

FACET Additives

- Overview of FACET Additives
 - Additive Assessments using Pre-Installed Data (Example): Sunset Yellow (E110)
 - Additive Assessments using Pre-Installed Data (Exercise): Green S (E142)
- Application of Concentration Ranges (fixed or distributional) with occurrence data (Example): Sunset Yellow
- Questions, Discussion and Summing Up

Session 1: introduction to FACET



FACET FCM Overview

Dr. Seamus Kelly
Dr. Aileen Connolly
Creme Global
2014

Overview of FACET



- Objective:
 - Create a Food Chemical Exposure Surveillance System which covers representative regions of the EU
 - Exposure to Additives, Flavourings and Material Substances
 - Interest to Industry
- Duration: 2008 – 2012
- 20 collaborative partners across EU

What can FACET do for FCMs?



1. Populate a database of substance migration in foods
2. Estimate dietary exposure to food packaging substances
3. Break down contribution to exposure by:
 - a. Food type
 - b. Packaging type
4. Estimate exposure to a new packaging type brought to market

Product Safety?



- Different Approaches can be used to estimate concentration levels (Estimated Daily Intake (EDI)) of the migrant in the food
- Once EDI is calculated then it can be compared to a Tolerable Daily Intake (TDI). If $EDI < TDI$, then the product is safe. Otherwise, further testing is required.

Exposure: Method 1



- Method 1:
 - Assume 100% migration of the migrant
 - Assume that every day an adult person consumes 1kg of food packaged in a 1dm³ cube with a SA of 6 dm²
 - EDI(mg/person/day) = 1kg food/person/day * Migration (mg/kg food)

Exposure: Method 2

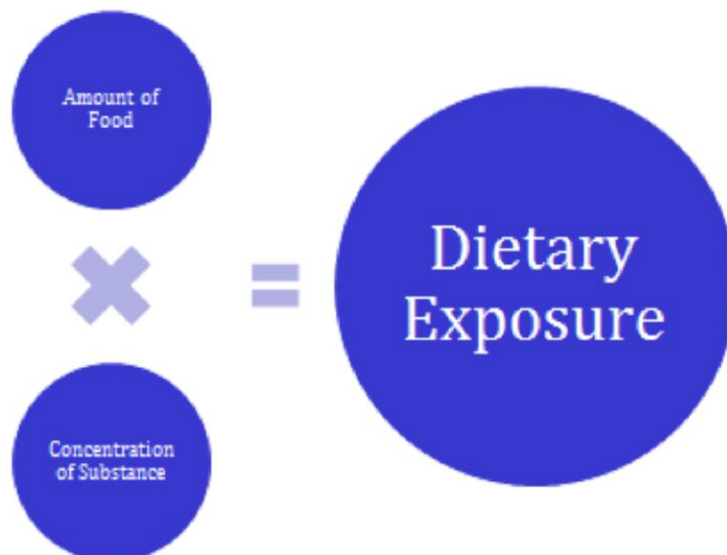


- Method 2: FACET
 - Diffusion model used to estimate migration of migrant into food
 - Consumption diaries used to estimate levels of consumption of different foods
 - EDI(mg/person/day) = Consumption(foodA) * Migration of substance from PackX into foodA / Subject Bw.

Probabilistic Dietary Exposure

BASIC PRINCIPLES

Basic Principle



Data Inputs: Consumption Data



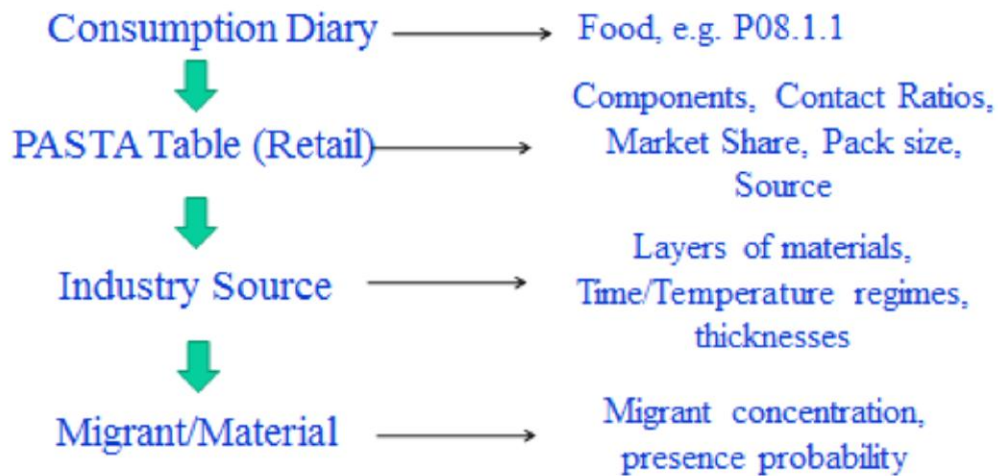
- Food Diaries
 - Countries
 - Finland, France, Hungary, Ireland, Italy, Poland, Portugal, UK.
 - Subject Diaries
 - SubjectIdCountry, Gender, Age, Weighting
 - Consumption Diaries
 - SubjectId, Food, Frequency, Amount

Other Data Inputs



- Retail Data: Contact Ratios, Pack Sizes, Market Shares
- Industry Data: Material Layers, Time/Temperature Regimes, Thicknesses
- Migrant Data: Migrant Concentrations in Materials, Presence Probabilities

Linking Foods to Migrants



Migration Model for Multi-Layer Packaging



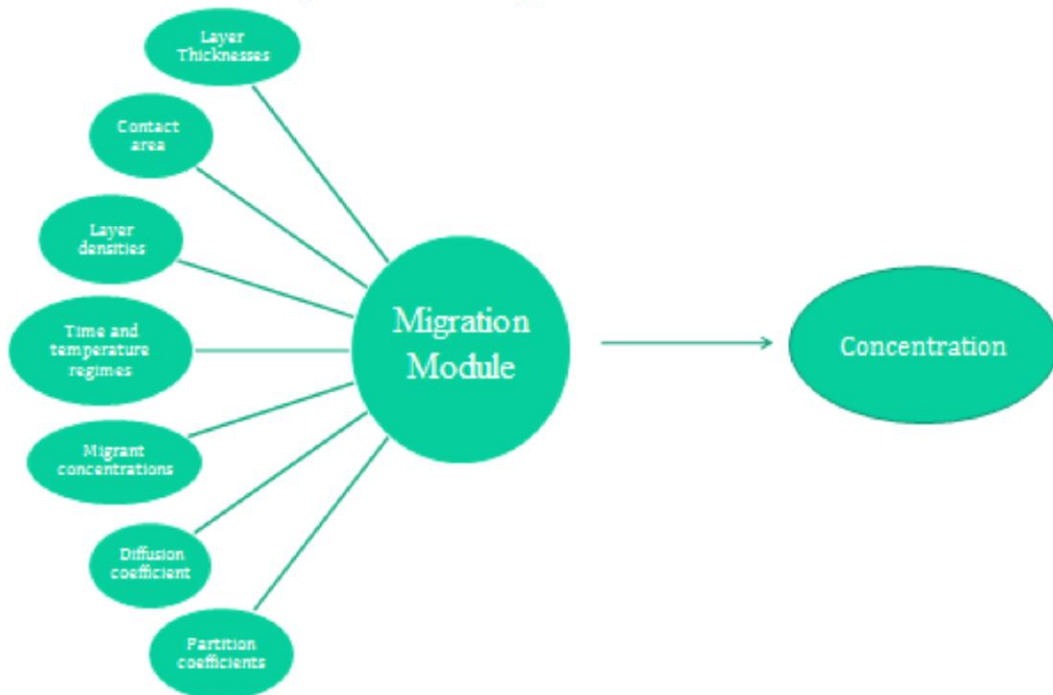
- Model is one-dimensional PDE that outputs the concentration of a migrant in food as a function of time
- Model is based on Fick's second law of diffusion.

Packaging Structure



Layer 1 (Outside Layer)
Layer 2
Layer 3
...
Layer N (Food Contact Layer)
Food

Inputs into Migration Model



Also Required



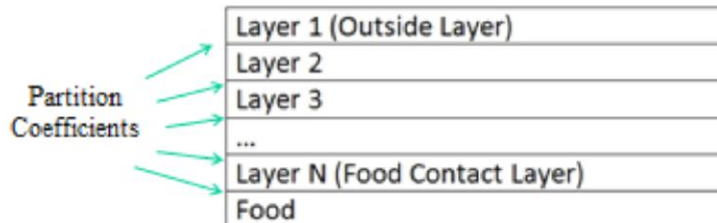
- Diffusion Coefficient for each material/migrant combination = $f(A_p, \tau, M_w, T)$
 - A_p, τ are diffusion coefficient parameters
 - M_w is the molecular weight of molecule
 - T is the temperature
 - f is Piringer's Formula

Also Required



- Partition coefficients for each material/material and material/food interface
- Densities of foods and materials

Packaging Structure



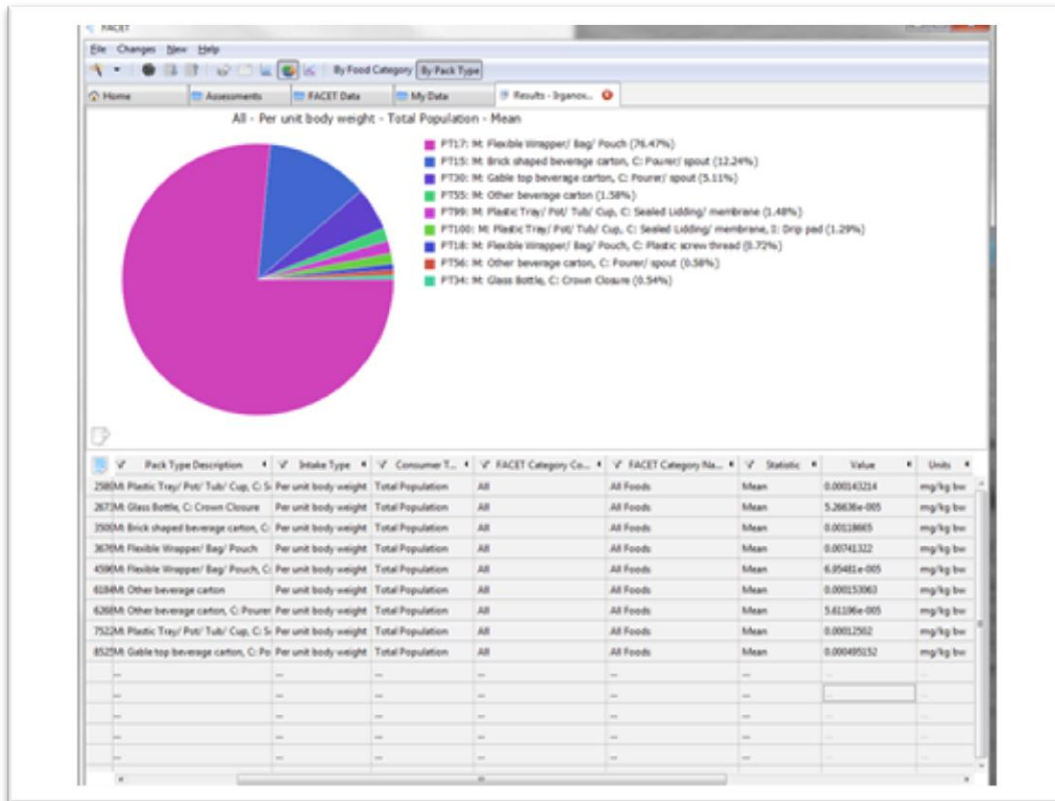
Determining Exposure




- To determine exposure at each event:

$$\text{Exposure} = \sum_{\text{Food quantity consumed}} [\text{Food Amount}] \times [\text{Concentration of Migrant}]$$

- Concentration is pre-calculated as a distribution; therefore MC simulations required.



Statistical Background



Statistical Background



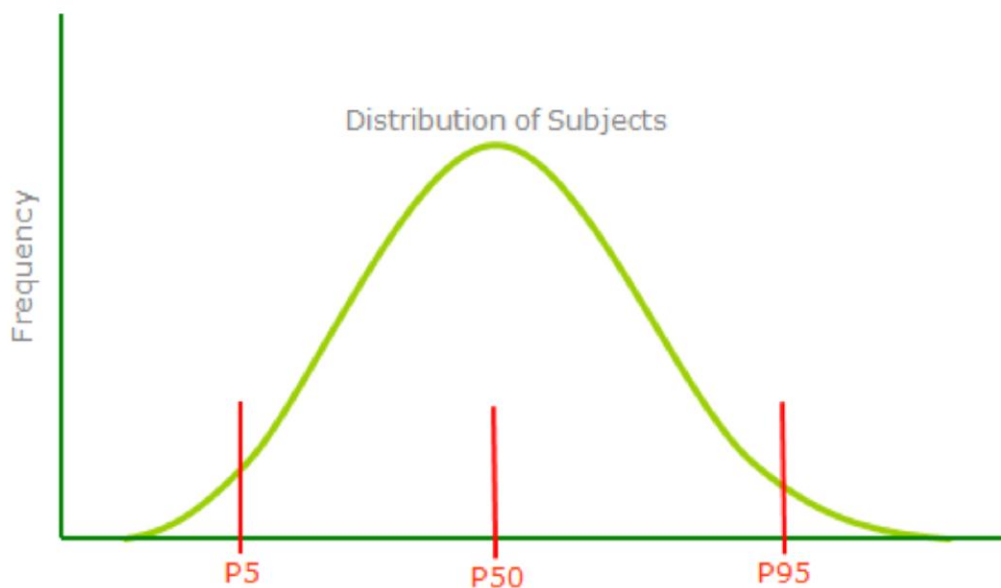
- Exposure is usually calculated in a population; therefore *variable*
- Generally a *distribution* of exposure is estimated, taking into account the variability in the population
- Once the distribution of exposure is calculated, it is described using various statistics

Exposure Statistics



- Mean: the arithmetic mean or average exposure in the population
- Percentile: Value of a variable below which a certain percent of observations fall
 - E.g. the P20 is the value below which 20% of the exposures fall
- In risk assessment, the upper percentiles are typically most important, e.g. the *P95 of exposure*.

Percentiles



Relevant Questions for an Exposure Assessment



- What is the mean exposure in the total population?
- What is the P95 of exposure?
- What is the mean exposure amongst consumers who consume that food?
- What is the P95 of exposure amongst food consumers?
- What is the acceptable/tolerable/recommended daily intake?

Session 2: FACET for food additives



FACET Additives Overview

Dr. Aileen Connolly
Dr. Seamus Kelly
Creme Global
2013

What can FACET do?

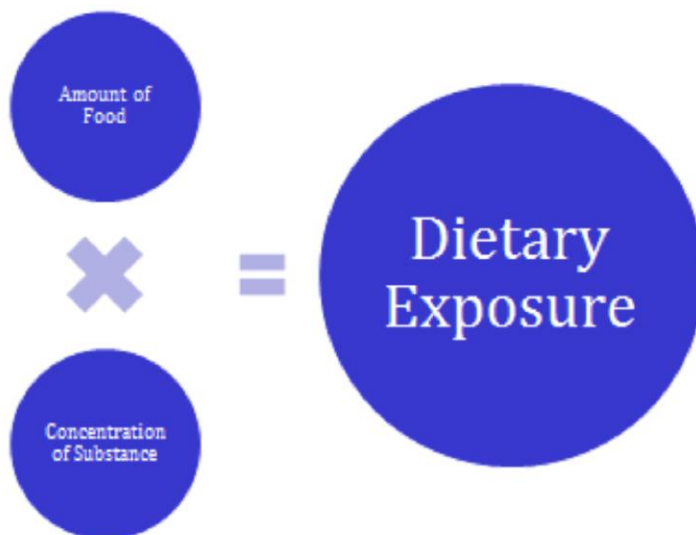


1. Estimate dietary exposure to food additives using food consumption data combined with:
 1. Maximum Permitted Levels
 2. Industry data
 3. Occurrence data
2. Break down contribution to exposure by food type
3. Estimate exposure using a new set of concentration data

Probabilistic Dietary Exposure

BASIC PRINCIPLES

Basic Principle



Consumption Data



- **Food Diaries**
 - **Countries**
 - Finland, France, Hungary, Ireland, Italy, Poland, Portugal, UK.
 - **Subject Diaries**
 - SubjectId, Country, Gender, Age, Weighting
 - **Consumption Diaries**
 - SubjectId, Food, Frequency, Amount

Diary Sizes

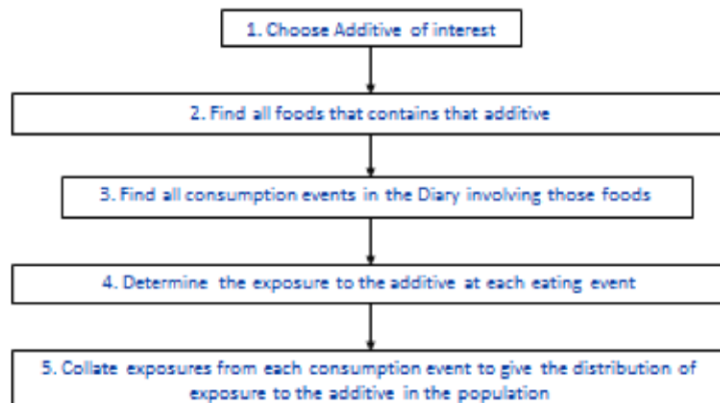


Country	Subjects	Consumption Events
France	4,079	541,453
Italy	3,322	322,178
UK (16-64)	1,631	298,086

Dietary Surveys



Additive Exposure Algorithm



FACET Food Codes



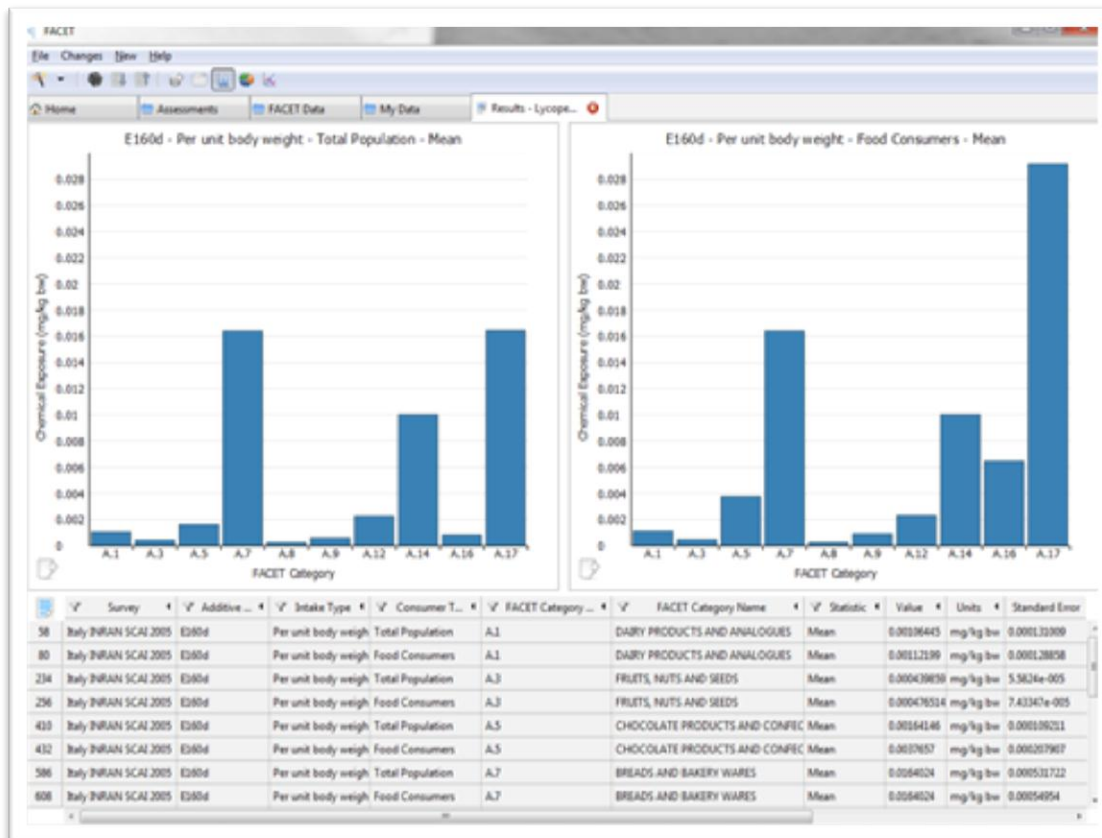
- System is tiered, e.g.
 - A.05: Chocolate products and confectionary
 - A.05.1: Cocoa and chocolate products
 - A.05.1.2: Cocoa-based spreads
 - A.05.2: Confectionary including hard and soft candy
 - A.05.2.1: Glucose syrup-based confectionery
 - A.05.2.2: Sugar confectionary
- More information specific to food can be included via additive flags:
 - Nutritional information (e.g. Low fat, sugar reduced)
 - Topping (e.g. Chocolate topping, whipped cream)
 - Coating
 - Filling

Concentration Sources



$$\text{Exposure} = \sum_{\substack{\text{Food quantity} \\ \text{consumed}}} [\text{Food Amount}] \times [\text{Concentration of Additive}]$$

- Regulatory data
 - Maximum Permitted Levels (MPLs)
- Industry Data
 - Typical Min
 - Typical Max
 - Extreme Min
 - Extreme Max
 - Fitted distribution
- Can be assessed with or without probability of occurrence



Relevant Questions for an Exposure Assessment



- What is the mean exposure in the total population?
- What is the P95 of exposure?
- What is the mean exposure amongst consumers who consume that food?
- What is the P95 of exposure amongst food consumers?
- What is the acceptable/tolerable/recommended daily intake?

Session 3: FACET for food flavourings



Expert Models for Decision Makers™

FACET Flavours Overview

Dr. Seamus Kelly
Dr. Aileen Connolly
Creme Global
October 2014

Flavourings: What can FACET do?



1. Estimate dietary exposure using screening methods.
2. Estimate dietary exposure to Added and Natural flavourings using a more refined approach.

Flavouring Assessments

Approach 1

Using Screening Methods

Screening Methods



- Theoretical Added Maximum Daily Intake Method (TAMDI)
- Modified TAMDI (mTAMDI)
- Single Portion Exposure Technique (SPET)
- Added Portions Exposure Technique (APET)

Screening Method (mTAMDI)

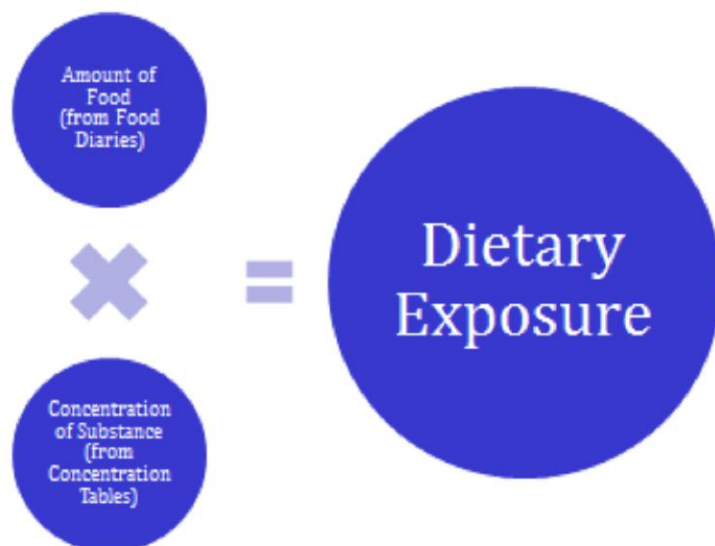


Food Groups	TAMDI Consumption (g/day)	Average Use Level (AUL) (mg/kg)	mTAMDI Exposure (mg/day)
Food	133.4	3.1	4.134
Beverages	324	0.6	0.194
Exceptions:			
a) Candy	27	9	0.243
b) Condiments	20	0.1	0.002
c) Alcoholic beverages	20	0.9	0.0018
d) Soups	20	0.6	0.012
e) Other exceptions	2	0.1	0.0002
			1.867

Approach 2

Using a Diary Driven Approach

Basic Principle



Consumption Data



- **Food Diaries**
 - **Countries**
 - Finland, France, Hungary, Ireland, Italy, Poland, Portugal, UK.
 - **Subject Diaries**
 - SubjectId, Country, Gender, Age, Weighting
 - **Consumption Diaries**
 - SubjectId, Food, Frequency, Amount

Diary Sizes



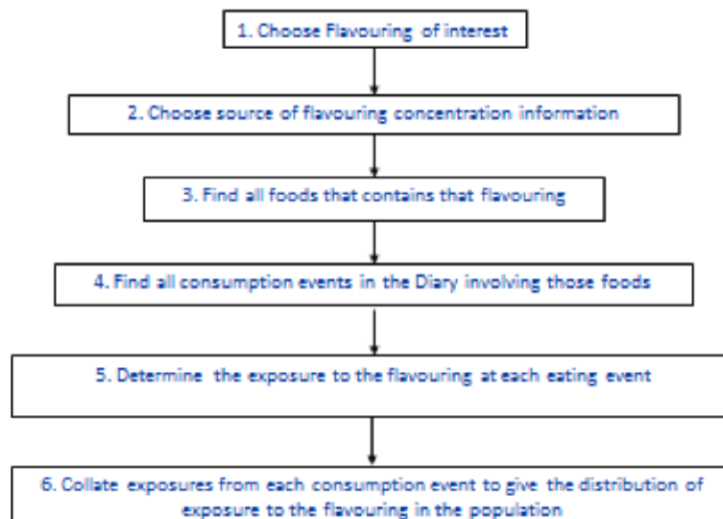
Country	Subjects	Consumption Events
France	4,079	541,453
Italy	3,322	322,178
UK (16-64)	1,631	298,086

Concentration Data



- Eight possible sources of concentration data for added flavourings (2700+ flavourings):
 - FEMA
 - IOFI-JECFA 2006, IOFI-JECFA 2007, IOFI DG SANCO 2010, IOFI-FACET 2010
 - CoE
 - EFSA
 - Young et al.
- For naturally occurring flavourings, the TNO database was used

Flavouring Exposure Algorithm



Added Flavourings

Three Assessment Types

- **Basic**
 - Covers all 2700 substances
 - All eating events involving foods with non-zero concentration for that substance are used
- **Intermediate**
 - Covers all 2700 substances
 - All eating events with non-zero concentrations for that substance considered except
 - Foods with flag “Without Added Flavouring”
 - Foods with “Unprocessed” packaging flag in food category “Fruits, Nuts and Seeds”

Three Assessment Types



- Refined
 - All eating events involving foods with non-zero concentrations are used and the full FACET flavouring flag system is used to determine exposure

Example of Added Flavouring Assessment



Event	Subject	Day	Food	Amt (g)	FL 6	FL 7
1	1324	1	F14.4.1	100	1: Without	-3: NFI
2	1324	1	F.14.4.1	250	2: With	-3: NFI
3	1324	2	F.14.4.1	150	19: Raspberry	18: Strawberry
4	1324	2	F.14.4.1	150	6: Vanilla	-3: NFI
5	1324	2	F.14.4.1	200	-3: NFI	-3: NFI

Food	Substance	Typical Conc (mg/kg)	Upper Conc (mg/kg)
F14.4.1	Raspberry Ketone	0.05	0.1
F.14.4.1	Vanillin	0.1	0.15

Comparing Assessments



- **Basic**
 - Flags not used
 - All 5 eating events have exposure to both Raspberry and Vanillin
- **Intermediate**
 - Events with flag value “Without Added Flavourings” are ignored
 - Only events 2-5 are considered

Refined Assessment



- Full flags system is used
- Extra Probability of Addition table required

Substance	Food	Flag Value	Prob of Addition	Refined Conc Level
Raspberry Ketone	F14.4.1	11: Forest Fruits	0.9	
Raspberry Ketone	F14.4.1	18: Strawberry	0.5	
Raspberry Ketone	F14.4.1	19: Raspberry	0.8	
Vanillin	F14.4.1	6: Vanilla	0.7	0.12

Refined Assessment



- Refined
 - Only eating events with non-zero probability of addition value for one of its flags are used
 - Event 2 has exposure to both Raspberry Ketone and Vanillin
 - Event 3 has exposure to Raspberry Ketone
 - Event 4 has exposure to Vanillin



Natural Flavourings

Natural Flavouring



- Here concentration values are calculated from TNO database
- Natural flavourings include:
 - Flavourings that exist naturally in the food
 - Flavouring that exists naturally in an ingredient in the food
- Total Dietary Exposure = Dietary Exposure (Added Flavourings) + Dietary Exposure (Natural Flavourings)

Relevant Questions for an Exposure Assessment



- What is the mean exposure in the total population?
- What is the P95 of exposure?
- What is the mean exposure amongst consumers who consume that food?
- What is the P95 of exposure amongst food consumers?
- What is the acceptable/tolerable daily intake?

Exercises



FACET Workshop Exercises

"Exercises for FACET software"

JRC

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1 Document Metadata

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2 Exercises

This section contains exercises which present the user with an opportunity to become familiar with the functionality of the FACET software in the areas of packaging, flavourings, and additives.

2.1 Exercises: Food Contact Materials

2.1.1 Exercises: Running a Basic Packaging Assessment

Run a Packaging Assessment satisfying the following criteria:

- (i) Substance: 1334
- (ii) Pack Types: All Pack Types
- (iii) Foods: All Foods
- (iv) Survey: UK 19-64
- (v) Select Males between the ages of 20 and 25
- (vi) Assessment Name: Substance: 1334 – Survey: UK_19-64 – Packs: All – Foods: All – Loyal: Yes
- (vii) Select “With consumer loyalty”

2.1.2 Exercises: Working at Lowest Tier

Run a Packaging Assessment (at the lowest tier) satisfying the following criteria

- (i) Substance: 1334
- (ii) Pack Types: All
- (iii) Food Categories: Main driver from Exercise 2.1.1
- (iv) Survey: UK NDNS 2000 19-64
- (v) Loyalty: With
- (vi) Use SetOff: No

2.1.3 Exercises: Examining Results

In the first exercise the assessment “Substance: 1334 – Survey: UK_19-64 – Packs: All – Foods: All – Loyal: Yes” was created. Using the outputs from this assessment complete the following tasks.

- (i) Download the bar chart broken down “By Food Category” described as follows: “Per unit body weight” for “Total Population”
- (ii) Download the bar chart broken down “By Food Category” described as follows: “Per unit body weight” for “Food Consumers”
- (iii) Download the data broken down “By Food Category”
- (iv) Download the pie chart broken down “By Food Category” described as follows: “Per unit body weight” for “Total Population”
- (v) Download the bar chart broken down “By Pack Type” described as follows: “Per unit body weight” for “Total Population”
- (vi) Download the Report summarising the assessment outputs.

2.1.4 Exercises: Entering extraction/migration data

Use the “New Packaging Wizard” and “New Assessment” tools to initially establish the concentration levels of the given substance in the chosen foods in (i) and hence run an exposure assessment for the chosen country in (ii).

- (i) Existing Substance in Non-Metal Pack Type
 - a. Metal: No
 - b. Existing Substance: Yes
 - c. Substance: 1334 (styrene)
 - d. Include set-off: No
 - e. Surface / Volume: 0.6
 - f. (Pack) Type: Plastic tray/pot/tub/cup
 - g. Material Code: M.15.1 Non-expanded PS
 - h. Concentration: 10
 - i. Thickness: 250
 - j. Food Categories: P.17.1.1 Spoonable Yogurt
 - k. Pack Size: 250
 - l. Time: 1 month
 - m. Temperature: 40 degrees centigrade
 - n. Table Name: Substance: 1334 – Metal: No – SetOff: No – Food: Spoonable Yoghurt

- (ii) Use the results in (i) to run a Packaging Assessment satisfying the following criteria:
- a. Pack Types: All
 - b. Food Categories: P.17.1.1 Spoonable Yoghurt
 - c. Survey: UK NDNS 2000 19-64
 - d. Assessment Name: Substance: 1334 – Metal: No – SetOff: No – Food: Spoonable Yoghurt
 - e. Consumer Loyalty: Without
 - f. Use SetOff: No

2.2 Exercises: Food Flavourings

2.2.1 Exercises: Running a Basic Flavourings Assessment

Run a Flavouring Assessment satisfying the following criteria:

- Substance: Trans-2-hexenal (FL-no: 05.073)
- Concentration Data: EFFA
- Foods: All (but investigating top 3 contributors)
- Survey: Italy INRAN SCAI 2005
- Gender: Both
- Ages: 20 – 40 years
- Assess Using: Typical use levels
- Exclude foods without added flavourings: No
- Exclude unprocessed fruits, nuts and seeds: No
- Use probability of addition data: No
- Flavouring Source: Added and Natural
- Advanced Options: No
- Observe outputs/results in the report and graphs

2.3 Exercises: Food Additives

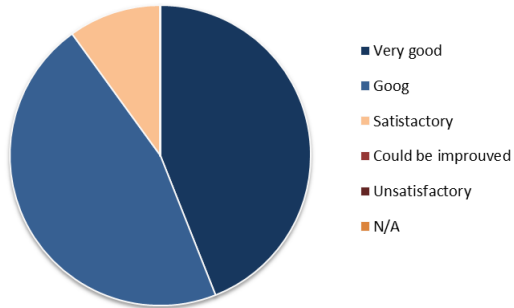
2.3.1 Exercises: Running a Basic Additives Assessment

Run an Additive Assessment satisfying the following criteria:

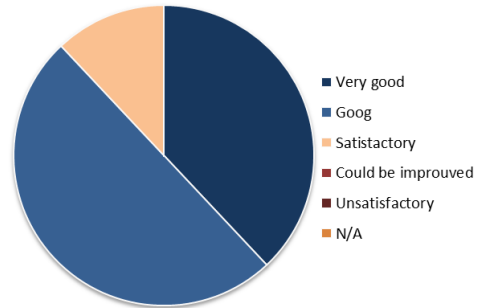
- Additive: Green S (E142)
- Foods: Selected Foods ('Non-Alcoholic Beverages', 'Alcoholic Beverages', 'Salts, spices, sauces & soups' and 'Breads & Bakery Wares')
- Survey: UK 19-64
- Gender: Both
- Ages: 20-22
- Assess Using: MPL
- Consumer Loyalty: No
- Include Occurrence Data: No
- Advanced Options: No

Annex 1: Feedback from participants – customer satisfaction

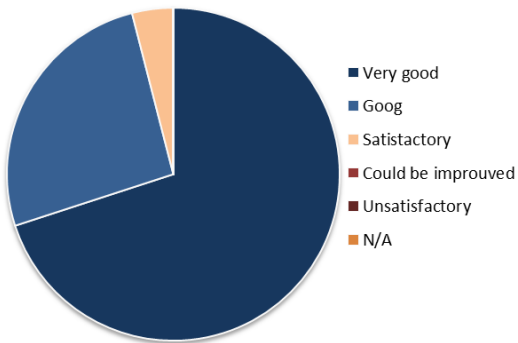
Programme and objectives



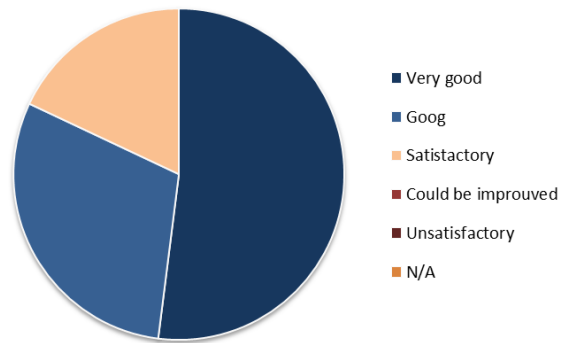
Contents, quality of presentation



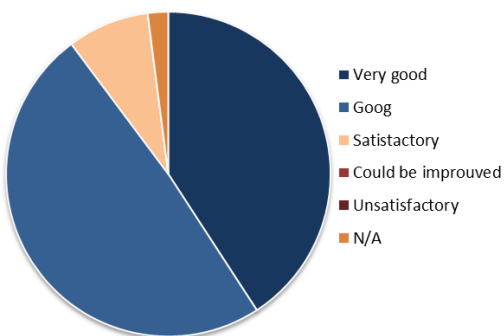
Trainers competence



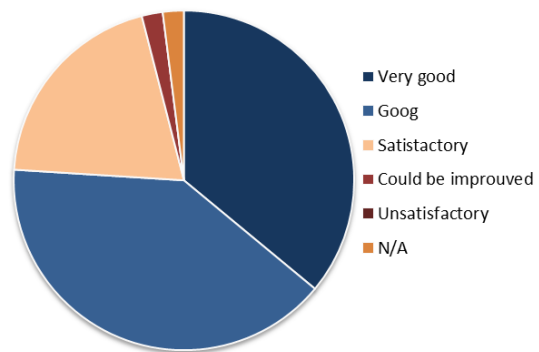
Interaction with trainers



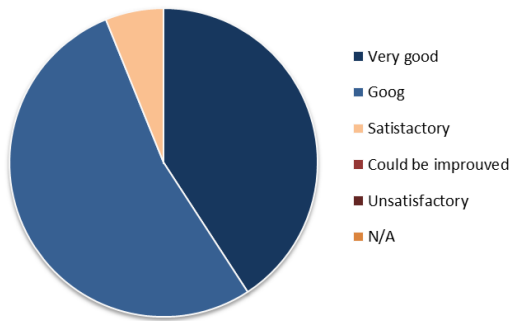
Balance between sessions



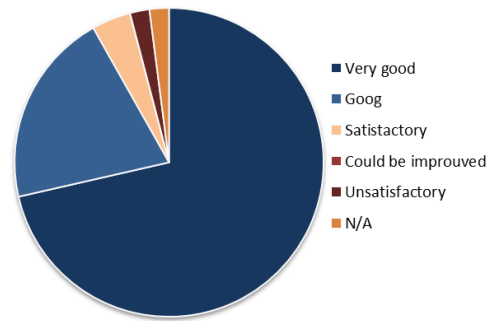
Supporting material



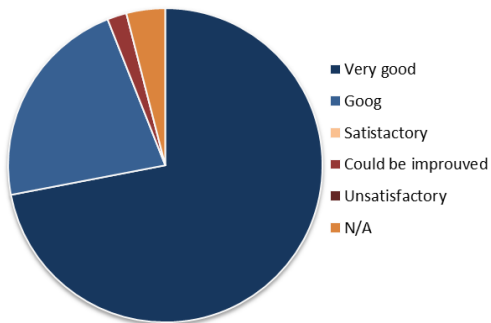
Overall evaluation



Online registration



Transport and venue



Note: it was very appreciated that industry people were also allowed to attend this training as well

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