



FACET Exposure Assessment Tool

User Manual

Version 2.0.6

December, 2013



Contents

System Requirements	4
Release Notes.....	4
Overview.....	5
Data Structures.....	6
Home.....	7
Assessments	8
Organising Assessments	10
Creating a new folder.....	10
Renaming a folder.....	11
Deleting a Folder.....	11
Renaming an Assessment	11
Deleting an Assessment	12
Viewing the Report	12
Viewing Graphs	12
Viewing Graphs	13
Viewing Data Only	17
Viewing All Results.....	18
Running an Assessment	19
Select Assessment Type.....	21
Select Substance.....	21
Searching for a Substance	22
Flavourings	22
Additives	23
Packaging Migrant	24
Search Results.....	25
Using Custom Concentration Data	26
Select Concentration Data.....	26
Select Pack Types	27
Food Categories	28
Select Survey	32
Select Population Filters	34
Assessment Options	35
Flavouring Assessment Options	36
Additive Assessment Options	37
Packaging Assessment Options	38
Advanced Options.....	39
Assessment Summary	40
FACET Data	42
Flags	43
Food Categories	43
Migration Information	46
Substances.....	47
Flavourings	48
Screening Calculations.....	51

Additives	51
Packaging.....	55
Surveys.....	57
My Data	59
Managing Data.....	59
Navigating about the data manager.....	59
Creating a new folder.....	60
Renaming a folder.....	60
Deleting a folder	60
New Table Wizard	61
The Data Editor.....	61
Insert Row	62
Delete Row.....	63
Entering data	64
Advanced Packaging Interface	67
New Pack Type	68
Metal Pack Type	77
Known Issues	85
Troubleshooting.....	85
Restart the software.....	85
Close FACET using the Task Manager	85
Uninstall and reinstall FACET.....	86
Failing all of the above	86

System Requirements

This software will run on machines using the Microsoft Windows XP®, Windows Vista®, or Windows 7® operating systems. The user must have administrator privileges on their PC to install this software.

Approximately 1GB of disk space is required for installation of the software. A processor with at least 1GHz clock speed and 1GB of RAM is recommended.

For optimum use of the software, it is recommended to use a display with resolution of 1024 x 768 or higher.

Release Notes

This software is the final implementation of the workflow, features, and functionality for the FACET exposure assessment tool. This workflow has been refined and modified over time based on consortium feedback from FACET versions 1.0 (January 2010), 1.2 (May 2010), 1.4 (October 2010), 1.5 (April 2011), 1.6 (February 2012), 1.7 (August 2012), 1.8 (October 2012), 1.9 (November 2012), 2.0 (August 2013), 2.0.6 (November 2013) . The software contains all databases and models gathered and developed over the course of the FACET project.

Overview

The software is implemented in a four panel layout. These four panels, referred to as “tabs”, are:

- **Home:** dashboard providing program status and basic program information.
- **Assessments:** interface to view results from completed assessments or the status of assessments currently running.
- **FACET Data:** interface to view non-sensitive data that has been pre-installed in the software.
- **My Data:** interface to view data that the user has loaded into the FACET program.

On starting the software, you will be presented with the “Home” tab.

You can navigate between tabs by clicking on the tab name (“Home”, “Assessments”, “FACET Data”, “My Data”) near the top left of the program window.

By default the program window opens to a default size. You can resize the window to the desired size, though to ensure adequate display of all features, there is a minimum allowed size for the window.

Data Structures

The FACET software supports a number of probabilistic data structures in the form of parametric and empirical distributions. In general, these can be used in place of point values for inputs such as chemical concentrations, contact areas, etc. A table of the possible options is below.

Distribution Type	No Of Arguments	Arguments	Example1
Uniform Distribution Discrete	Any	Comma separated values	choice(0, 1, 1, 2, 3, 5, 8, 13)
Weighted Distribution Discrete	Any	Comma separated values	weighted(0.2, 3.14, 0.2, 1.618, 0.6, 2.718)
Uniform Continous Distribution	2	Min, Max	uniform(1, 5)
Triangular Distribution	3	Min, Typical, Max	triangular(0, 1, 2)
Normal Distribution	2	Mean, S. D.	gaussian(23, 1)
Normal Distribution With Bounds	4	Mean, S. D., min, max	gaussian(23, 1, 22, 24)
Lognormal Distribution	2	Mean and S. D. of underlying normal	lognormal(74, 10)
Weibull Distribution	2	Shape, Scale	weibull(1, 1.5)
Chi Squared Disribution	1	Degrees of Freedom	chisquared(2)
Gamma Distribution	2	Shape, Scale	gamma(9, 0.5)

The “choice” distribution is used when a set of values are all equally likely.

The “weighted” distribution is used when different values occur with a given weight or frequency, in the form of (weight, value, weight, value,...). Note that the sum of the weights do not need to be less than zero or sum to one.

In general, these can be nested within each other, e.g. the individual elements of a weighted distribution can be composed of normal distributions: weighted(0.2, gaussian(2, 5), 0.8, gaussian(1,3)).

Home

The Home tab comprises:

- **Project Summary:** In the centre of the page is a brief summary of the FACET project.
- **Quick start buttons:** Below the project summary there are three quick start buttons. These are:
 - *Create New Assessment:* This launches the FACET Assessment Wizard that guides you through the steps required to perform an assessment. Clicking on this button is equivalent to clicking on the “New Assessment” button in the toolbar at the top of the screen.
 - *Go to FACET Data:* Clicking on this button will bring you to the “FACET Data” tab, where you can browse through non-confidential data built into the program. Clicking on this button is equivalent to clicking on the “FACET Data” tab.
 - *Go to My Data:* Clicking on this button opens the “My Data” tab, where you can browse and edit your own custom data for use in an assessment. Clicking on this button is equivalent to clicking on the “My Data” tab.

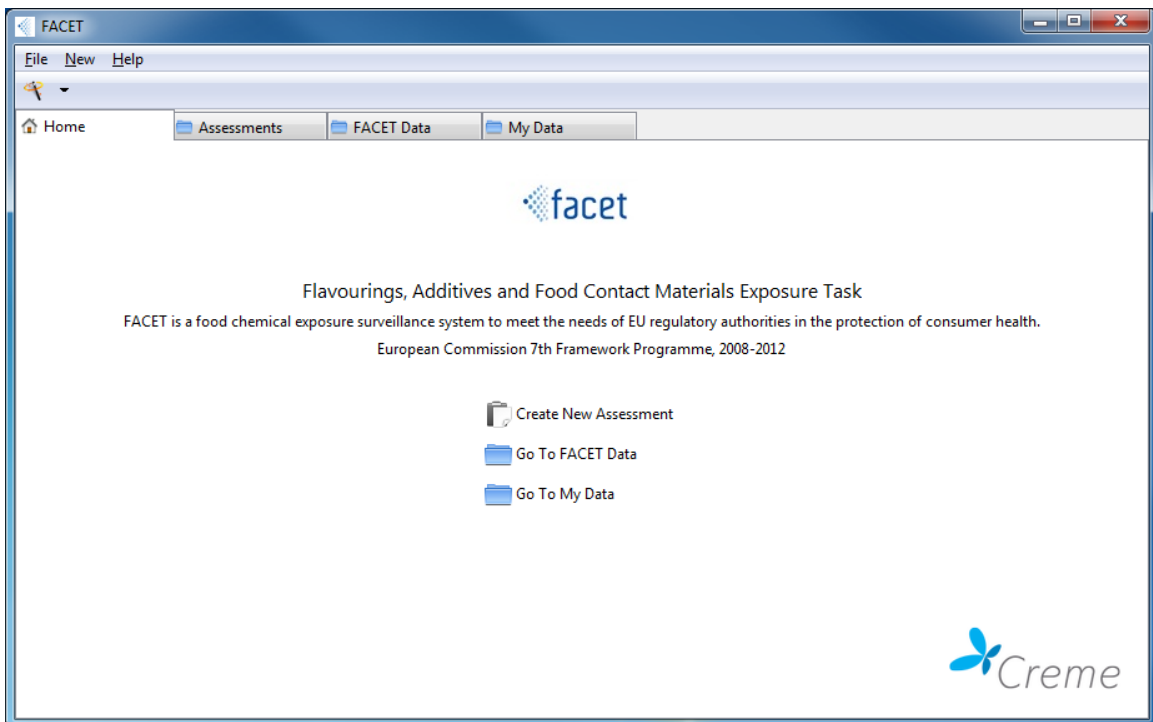


Figure 1: The Home Tab

Assessments

The assessment tab is where all of your assessments can be organised, and is similar to any file management system. The view is implemented in a three panel layout.

The left-hand pane shows a tree structure that shows how the user's folders are organised.

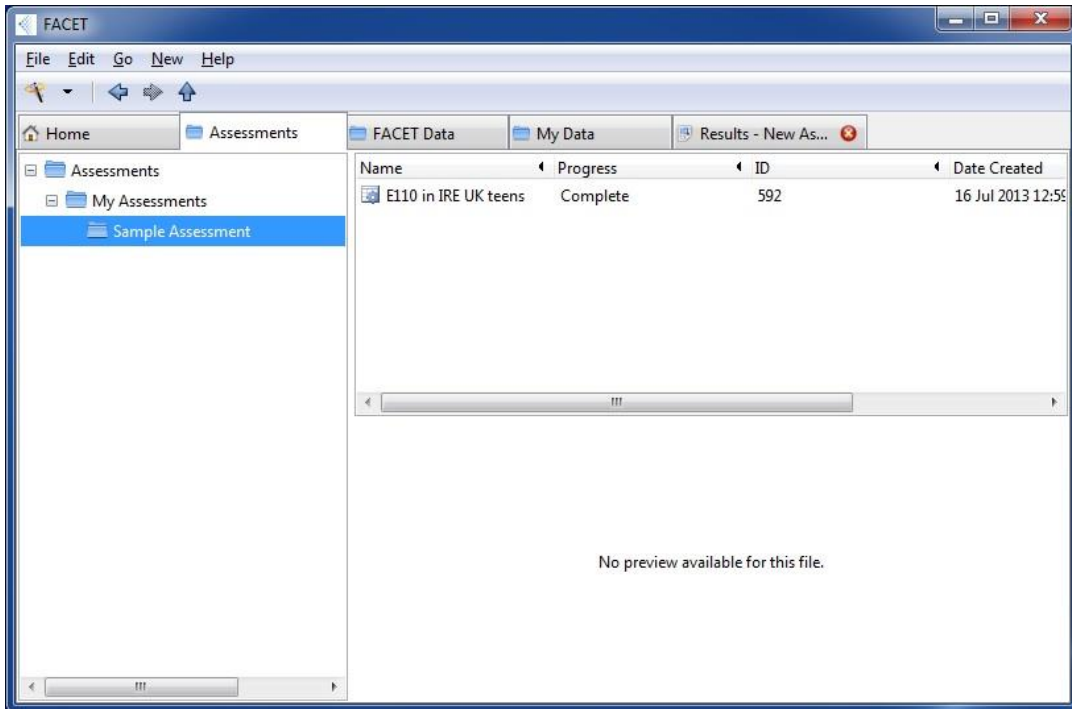


Figure 2: The assessment tab

The top right panel shows the contents of the folders, which are assessments. The assessments are presented in a list view, and the following fields are displayed:

- **Name:** The name given to the assessment by the user.
- **Progress:** This is a progress bar showing what percentage of the assessment has been completed.
- **ID:** The unique ID number of the assessment.
- **Date Created:** The date the assessment was run.
- **Date Accessed:** The date the assessment was last viewed.

Name	Progress	ID	Date Created
E110 in IRE UK teens	Complete	592	16 Jul 2013 12:59

Figure 3: List view of assessment

The bottom right panel provides the status and details of whatever assessment is selected in the top right pane. It also provides buttons that allow the user to view the results of the selected assessment (“View All Results”), view the graphs of the assessment (“View Graphs”) or view the report generated by the assessment (“View Report”). Descriptive fields appear in the assessment summary showing the following:

The screenshot shows the FACET software interface. The top panel displays a list of assessments with columns for Name, Progress, ID, Date Created, and Date Accessed. The selected assessment is 'Sample Ax: 9024 in French males < 20 yr old (All foods)' with ID 625, completed on 8 Aug 2012 12:35, and accessed on 16 Aug 2012 08:52. Below the list are buttons for 'View All Results', 'View Graphs', and 'View Report'. The bottom panel shows the 'Assessment Summary' for the selected assessment, with the following details:

Assessment Summary		
ID:	625	
Name:	Sample Ax: 9024 in French males < 20 yr old (All foods)	
Description:	Fitted distribution - lognormal	
Type:	Flavouring (FEMA)	
Substance:	9024 - Isopentyl acetate	
Survey(s):	<i>Name</i>	<i>Filtered Population Size</i> <i>Simulated Population Size</i>
	France INCA 2	740 740
Population Filters:	Gender: Male Age: between 0 and 20	
Date Submitted:	8 Aug 2012 12:35	
Software Version:	1.7b2	

Figure 4: Details of assessment

- **ID:** This is a unique identifier of the assessment within the program.
- **Name:** The name given to the assessment by the user.
- **Description:** Any further description the user included in the assessment.

- **Type:** The type of the assessment (Additive, Flavouring, or Packaging Migrant).
- **Substance:** The substance used in the assessment.
- **Survey(s):** The survey(s) used in the assessment, the number of subjects in the original survey (*Filtered Population Size*), and the number of subjects simulated (*Simulated Population Size*).
- **Population Filters:** Any population filters that may have been used in the assessment.
- **Date Submitted:** The date on which the assessment was performed.
- **Software Version:** The version of the software used to perform the assessment.

Organising Assessments

To navigate about the assessment manager, you can either:

1. Use the “Back”, “Forward”, and “Up” buttons in the tool bar.
2. Click on the folder whose contents you want to view in the folder tree in the left panel. The subfolders contained in a folder can be viewed by clicking on the plus symbol next to a folder in the left hand pane.
3. Double-clicking on the folder or assessment you want to view in the top right pane.

The folder structure in the left hand panel will expand or collapse to show where in the assessment manager you are currently viewing.

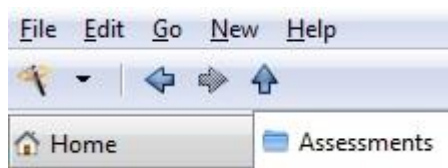


Figure 5: Back/forward/up arrows

Creating a new folder

1. To create a new folder, right click on where you want to create it in the top right pane and select “Create Folder”. Alternatively, select “Create Folder” from the file menu.
2. This will bring up a dialogue box into which you can enter the name of the new folder.
3. After entering the name of the new folder, click on “OK” and the new folder will be created.

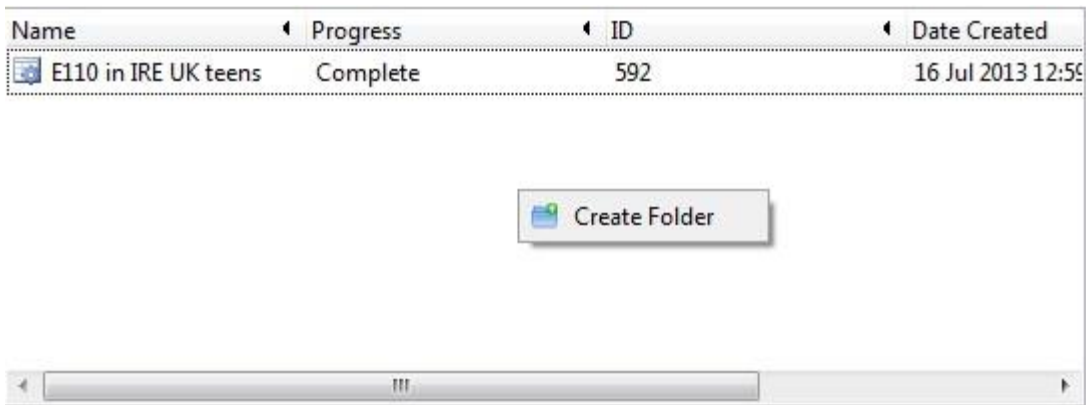


Figure 6: Creating a new folder

Renaming a folder

1. To rename a folder, right click on the folder you want to rename and select “Rename”. Alternatively, you can select the folder and choose “Rename” from the Edit menu.
2. This will bring up a dialogue box into which you can enter the new name of the folder. Enter the new name of the folder into the dialogue box and click on “Rename”.

Deleting a Folder

1. To delete a folder, right click on the folder you want to delete and select “Delete” from the context menu.
2. Alternatively, select the folder you want to delete and choose “Delete” from the Edit menu.

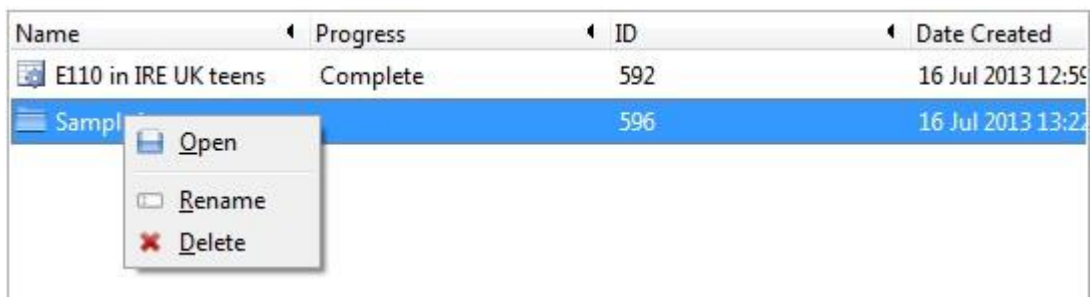


Figure 7: Renaming/deleting a folder

Renaming an Assessment

1. To rename an assessment, right click on the assessment you want to delete and select “Rename” from the context menu.

2. Alternatively, select the assessment you want to rename and choose “Rename” from the Edit menu.

Deleting an Assessment

1. To delete an assessment, right click on the assessment you want to delete and select “Delete” from the context menu.
2. Alternatively, select the assessment you want to delete and choose “Delete” from the Edit menu.
3. Note that if the assessment is running, you can still delete it.

Viewing the Report

To view the report generated by the software:

1. Navigate to where the assessment is located in the assessment manager and click on it.
2. A summary of the assessment will appear in the bottom right pane.
3. Click on the “View report” button in the top right hand side of the preview pane. This will bring up the report viewer, showing a summary of the report and some basic statistics.
4. To print the report, click on the “Print” button in the top right left hand corner of the report.
5. To save the report in PDF format, click on the “Export” button in the top left hand corner of the report.

Viewing Graphs

To view graphs and statistics generated by an assessment:

1. Navigate to where the assessment is located in the assessment manager and click on it.
2. A summary of the assessment will appear in the bottom right pane.
3. Click on the “View Graphs” button in the top right hand side of the preview pane. This will bring up the results viewer, showing graphs and statistics generated by the assessment.

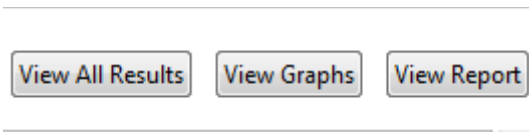


Figure 8: View report buttons

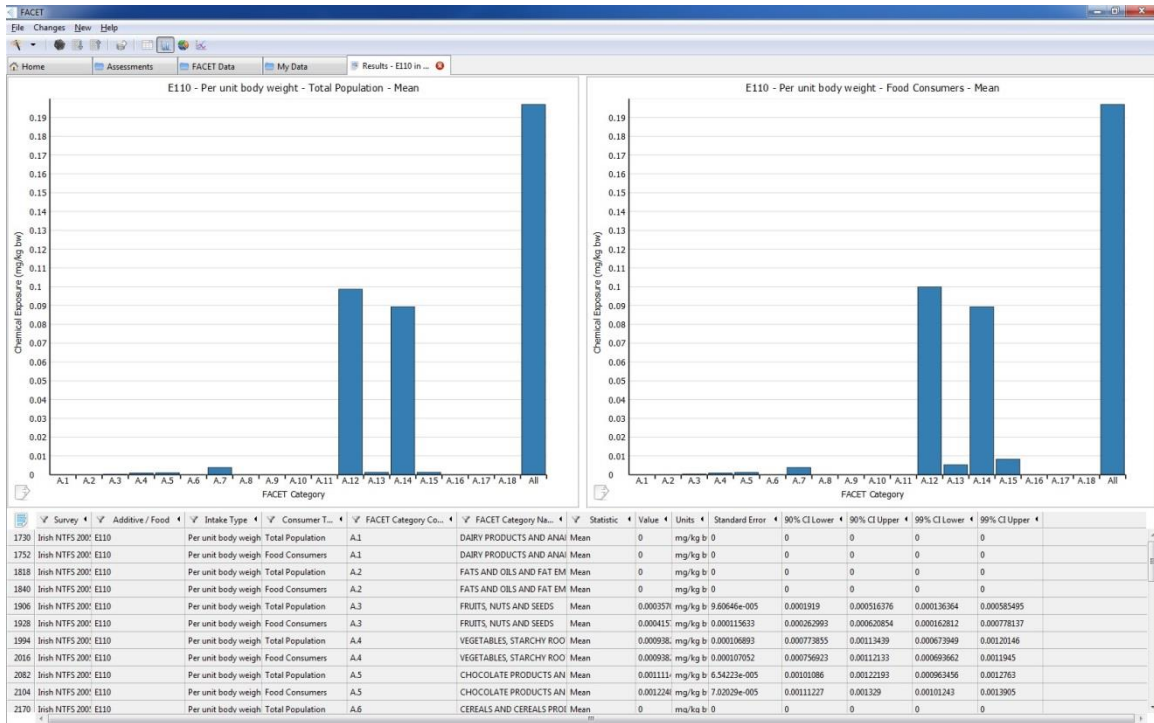


Figure 9: Results viewer –Column Chart and Data

There are four available views, three graphical views (column charts, pie charts, and distributions) and a data view. To toggle between the views click on the different graph icons or the data icon in the toolbar.

Viewing Graphs

By default, the assessment results appear with graphical views of the exposure assessments are presented above the data grid. The content of the graphs is controlled by the filters on the data grid fields.

To control the type of graph being displayed, click on the different graph icons in the tool bar. There are three graph types:



Column Chart: A chart with vertical rectangular bars with lengths proportional to the values that they represent. The level of exposure is on the y-axis and the FACET food category is on the x-axis.



Pie chart: A circular chart divided into sectors, illustrating proportion. The arc length of each sector is proportional to the quantity it represents. The chart is displayed with a legend on the right hand side, and only applies to the mean statistic in the total population.

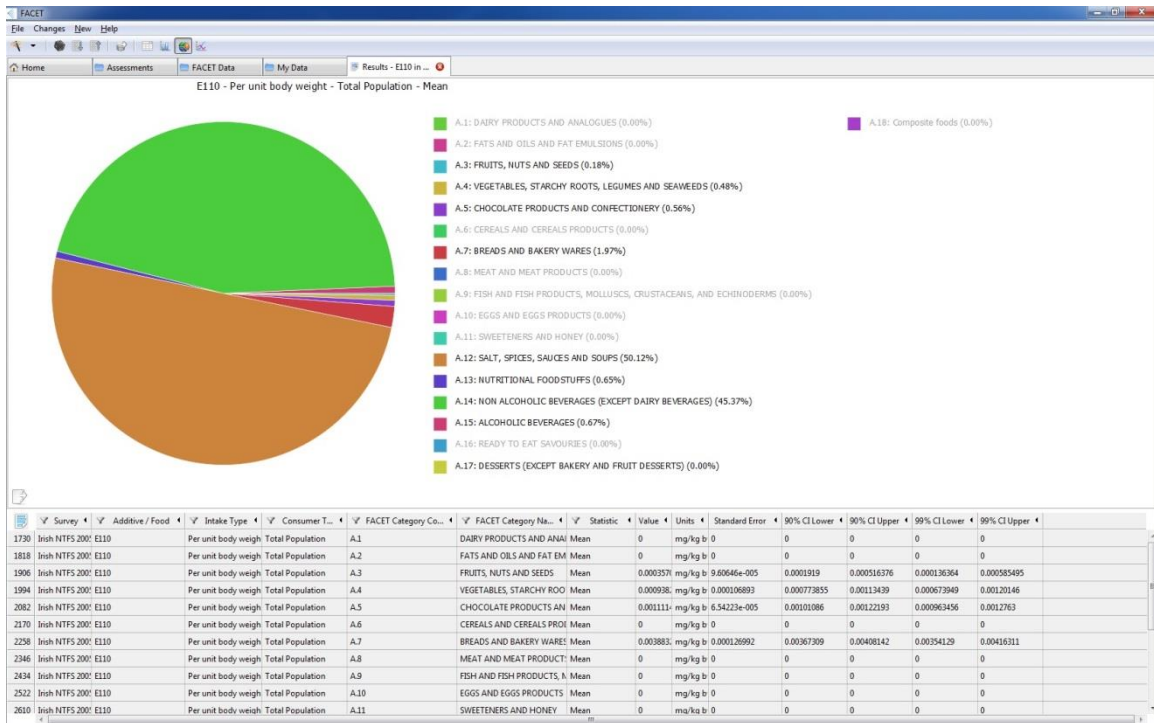


Figure 10: Results viewer – Pie Chart and Data



Distribution: There are two types of distribution charts, which can be selected from the “statistic” column in the data grid.

- **PDF:** Probability density function, which describes the relative likelihood for a random variable to occur at a given point (note that in cases when there is a constant amount of exposure for all subjects the range of the PDF will be 0 to 1e-06, purely for graphing purposes).

- **CDF:** Cumulative distribution function, which displays the probability that an exposure value will be found at a value less than or equal to a given number.

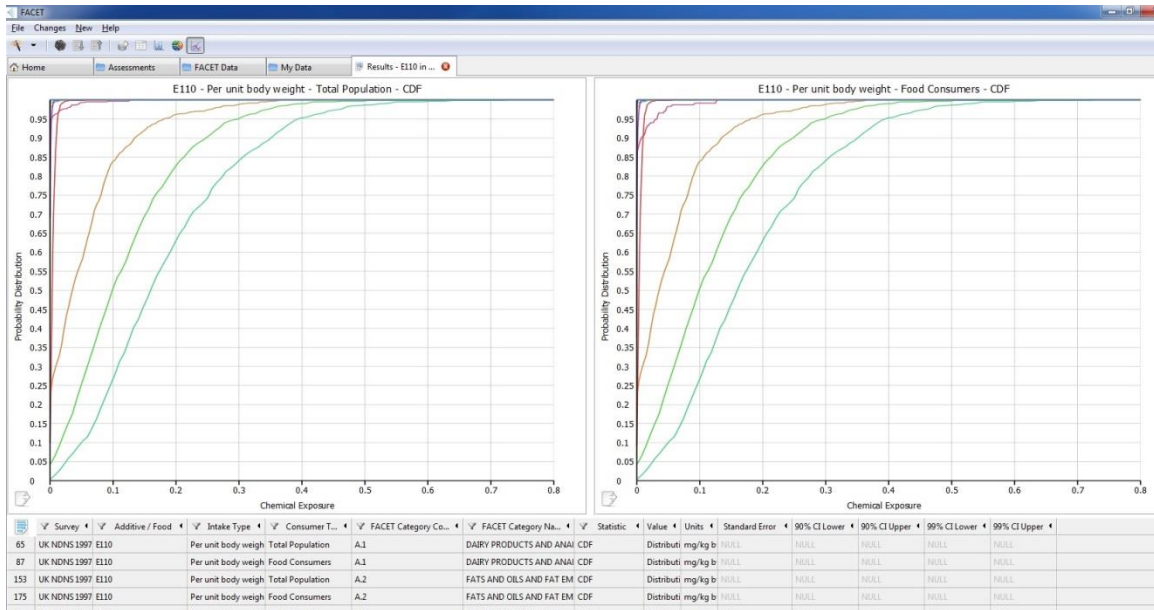


Figure 11: Results viewer: Line Graph and Data

To control what data appears on a selected graph there are filters in the headers of each column. Clicking on the header shows the available filters for that field. There are two filter types:

	Survey	Additive / Food	Intake Type	Consumer T...	FACET Category Co...	FACET Category Na...	Statistic	Value	Units	Standard Error
1730	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.1	DAIRY PRODUCTS AND ANAI	Mean	0	mg/kg bw	0
1818	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.2	FATS AND OILS AND FAT EM	Mean	0	mg/kg bw	0
1906	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.3	FRUITS, NUTS AND SEEDS	Mean	0.000357	mg/kg bw	9.60646e-005
1994	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.4	VEGETABLES, STARCHY ROO	Mean	0.000938	mg/kg bw	0.000106893
2082	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.5	CHOCOLATE PRODUCTS AN	Mean	0.001111	mg/kg bw	6.54223e-005
2170	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.6	CEREALS AND CEREALS PROI	Mean	0	mg/kg bw	0
2258	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.7	BREADS AND BAKERY WARE	Mean	0.003883	mg/kg bw	0.000126992
2346	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.8	MEAT AND MEAT PRODUCT	Mean	0	mg/kg bw	0
2434	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.9	FISH AND FISH PRODUCTS, N	Mean	0	mg/kg bw	0
2522	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.10	EGGS AND EGGS PRODUCTS	Mean	0	mg/kg bw	0
2610	Irish NTF5 2000	E110	Per unit body weigh	Total Population	A.11	SWEETENERS AND HONEY	Mean	0	mg/kg bw	0

Figure 12: Filters available.

- **Checkboxes:** This filter type applies to data that can be plotted simultaneously (e.g. FACET food categories).
- **Radio Buttons:** This filter type applies to data that cannot be plotted simultaneously (e.g. the Statistic column).

Each filter type is described in detail below:

- **Survey:** Used to alternate between different dietary surveys in a an exposure assessment. This has a radio button type filter.

- **Substance/Food:** Used to alternate between displaying exposure to a substance or intake of food. This has a radio button type filter.
- **Intake Type:** The type of exposure, which can be “Absolute” (measured in mg per day) or “Per unit body weight” (measured in mg per kilogram of bodyweight per day). This has a radio button type filter.
- **Consumer Type:** There are two possible consumer types, “Food Consumers” and “Total Population”. As these cannot be plotted together, each consumer type appears in a separate graph. This has a checkbox type filter.
- **FACET Category Code:** This allows you to decide which FACET food categories are displayed, by their numerical food code. This has a checkbox type filter.
- **FACET Category Name:** This allows you to decide which FACET food categories are displayed, by their food description. This has a checkbox type filter.
- **Statistic:** Shows what population statistic is plotted (e.g. mean, P90, P95 etc). This has a radio button type filter. When a distribution chart type is selected, this filter provides the option of displaying a PDF or CDF chart type.

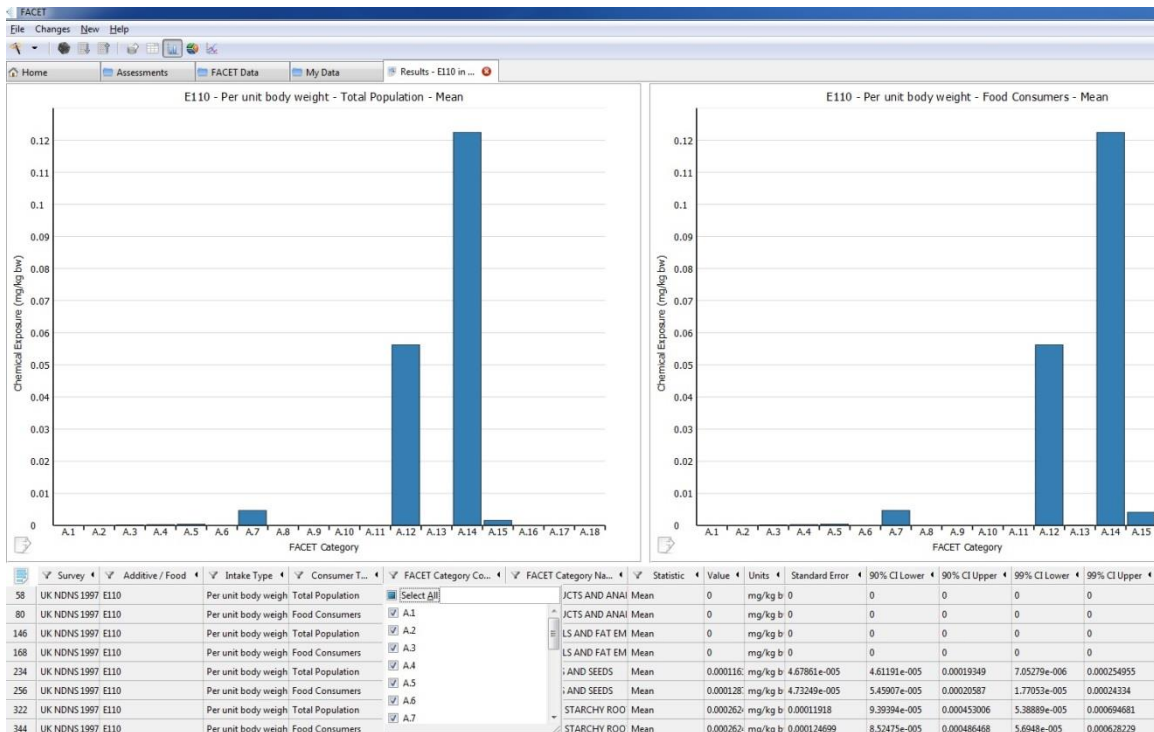


Figure 13: Column chart and data

There are additional fields that are used to display values in the chart type. These are:

- **Value:** The value(s) of exposure being displayed and plotted, according to the filter settings chosen.
- **Units:** The units of the value being displayed.

- Standard Error and Confidence Intervals:** These are used to display any confidence intervals calculated for the assessment, presented as upper and lower bounds. In the case of the standard error, this is a single value.

The values displayed can be exported as a CSV (Comma-Separated Values) file at any time by clicking on the export data icon located in the toolbar:



Data exported in CSV formatted can be opened later in a spreadsheet program like Microsoft Excel.

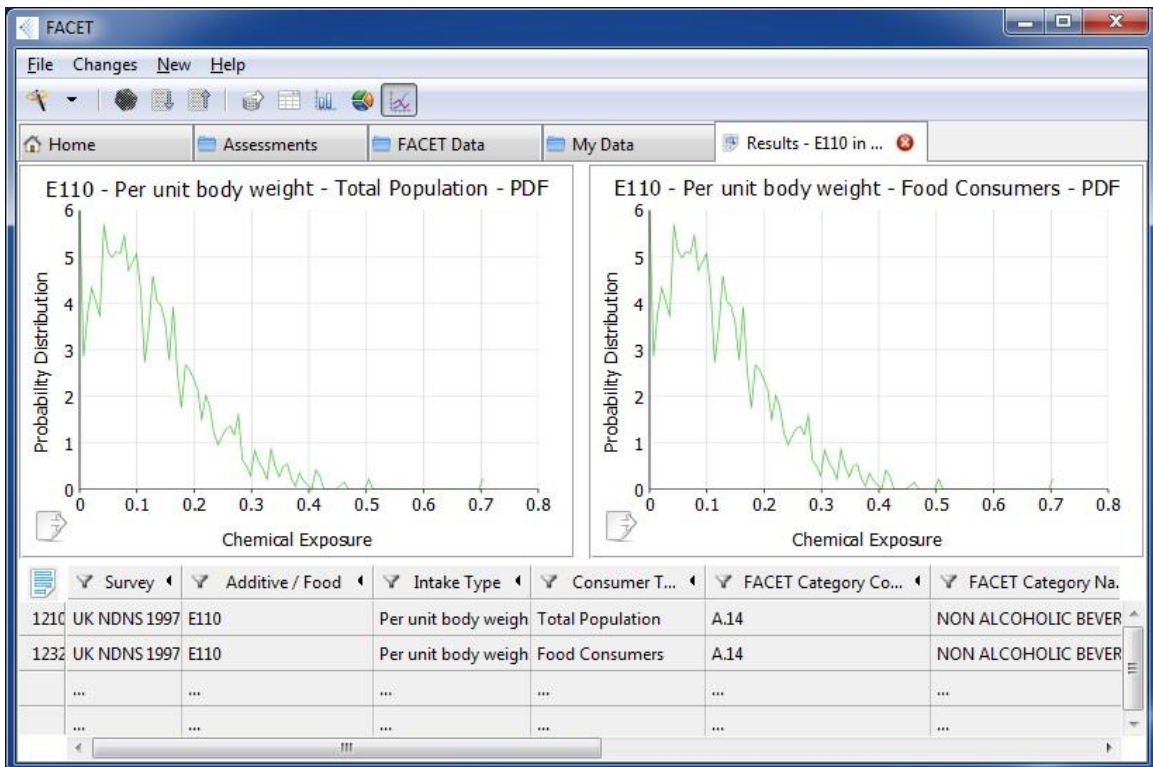


Figure 14: Probability density function chart and data

Viewing Data Only

To see the raw data calculated in an exposure assessment, click on the table icon in the toolbar. This will bring up a data-only view:



The table fields are the same as before, when the different graphs are being shown. However, since all the data is no longer being plotted, different combinations of data can be viewed simultaneously. Thus, all the filters are checkboxes when this view is selected.

The values displayed can be exported as a CSV (Comma-Separated Values) file at any time by clicking on the export icon located in the top left hand corner of the data grid:



Data exported in CSV formatted can be opened later in a spreadsheet program like Microsoft Excel.

	FACET Category Co...	FACET Category Na...	Statistic	Value	Units	Standard Error	90% CI Lower
1	A.1	DAIRY PRODUCTS AND ANAI	Count	1206		0	
2	A.1	DAIRY PRODUCTS AND ANAI	Percentage Consu	100	%	0	
3	A.1	DAIRY PRODUCTS AND ANAI	Mean	214.835	g	4.23178	
4	A.1	DAIRY PRODUCTS AND ANAI	Standard Deviatio	155.209	g	4.30623	
5	A.1	DAIRY PRODUCTS AND ANAI	Minimum	0	g	0.209841	
6	A.1	DAIRY PRODUCTS AND ANAI	Maximum	871.588	g	18.7314	
7	A.1	DAIRY PRODUCTS AND ANAI	P25	101.997	g	4.89288	
8	A.1	DAIRY PRODUCTS AND ANAI	P90	429.841	g	13.4244	
9	A.1	DAIRY PRODUCTS AND ANAI	P97.5	617.781	g	21.4082	
10	A.1	DAIRY PRODUCTS AND ANAI	CDF	Distributi	g	NULL	
11	A.1	DAIRY PRODUCTS AND ANAI	PDF	Distributi	g	NULL	
12	A.1	DAIRY PRODUCTS AND ANAI	Count	1206		0	
13	A.1	DAIRY PRODUCTS AND ANAI	Percentage Consu	100	%	0	
14	A.1	DAIRY PRODUCTS AND ANAI	Mean	0	mg	0	
15	A.1	DAIRY PRODUCTS AND ANAI	Standard Deviatio	0	mg	0	

Figure 15: Data only view

Viewing All Results

Results can be viewed in all food categories at the lowest, if this option is selected when the assessment is run (see “Running an Assessment” for details). If this option was checked when the assessment was run the button “View All Results” will be available. If this option was not chosen when the user ran the assessment, this option will be greyed out. To view results generated by an assessment:

1. Navigate to where the assessment is located in the assessment manager and click on it.
2. A summary of the assessment will appear in the bottom right pane.
3. Click on the “View All Results” button in the top right hand side of the preview pane (if available). This will bring up the results viewer, showing all statistics generated by the assessment at all food groups.

The results are outputted as a table that can be filtered as desired. Any result can be viewed simultaneously, so all fields have checkbox type filters. Each filter type is described in detail below:

- **Survey:** Used to alternate between different dietary surveys in a an exposure assessment.
- **Substance/Food:** Used to alternate between displaying exposure to a substance or intake of food.
- **Intake Type:** The type of exposure, which can be “Absolute” (measured in mg per day) or “Per unit body weight” (measured in mg per kilogram of bodyweight per day).
- **Consumer Type:** There are two possible consumer types, “Food Consumers” and “Total Population”.
- **FACET Food Code:** This allows you to decide which FACET food categories are displayed, by their numerical food code.
- **FACET Food Name:** This allows you to decide which FACET food categories are displayed, by their food description.
- **Statistic:** Shows what population statistic is plotted (e.g. mean, P90, P95 etc).

Running an Assessment

The New Assessment Wizard provides the workflow to set up a new exposure assessment. This can be selected from the file menu by selecting the “New” menu and then clicking on “New Assessment”. Alternatively, you can click on the wizard icon in the tool bar and select “New Assessment”, or select “Create New Assessment” in the home tab. When selected, the Assessment Wizard appears in a new window.

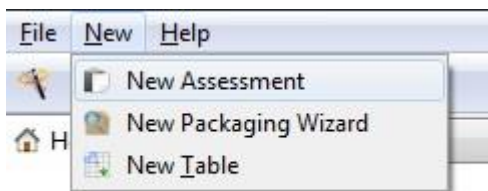


Figure 16: New assessment

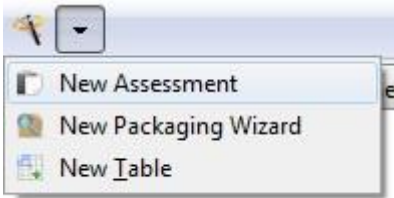


Figure 17: New assessment (2)

Depending on the assessment type, there are eight or nine steps to complete:

1. **Select Assessment Type:** Choose the type of assessment; flavouring, additive, or packaging migrant.
2. **Select Flavouring/Additive/Substance:** Choose substance to which exposure is to be estimated. This step also allows you to choose between using pre-installed FACET data or user-specified concentration data.
3. **Select Concentration Data:** For a flavourings assessment this also allows the user to choose which of the pre-installed sources of concentration to use.
4. **Select Pack Types:** For packaging assessments only. Choose all or specific packaging types to use in an assessment.
5. **Select Food Categories:** Choose all or specific food categories.
6. **Select Surveys:** Choose between different consumption surveys and specific ages or genders.
7. **Assessment Options:** Choose assessment name, description, output statistics and other options for the assessment.
8. **Assessment Summary:** Summary of selections for this assessment, and proceed to submit assessment.

You will be guided through these steps in sequential order. On successful completion of each step you can proceed to the next step by clicking the “Next” button at the bottom left of the program window. If you click the “Next” button without successfully completing the current step, a red “X” will appear next to that step to indicate it has not been successfully completed.

You can also navigate between the already completed steps by either:

- Clicking “Next” at the bottom right of the program window.
- Clicking “Previous” that appears in the bottom right of the Assessment Wizard window.
- Clicking the stage name buttons at the left hand of the program window.

It is not possible to proceed to a later step using these stage name buttons without having already completed all steps previous to this later step.

Select Assessment Type

In Step 1, you are required to specify whether you are going to perform an assessment using a flavouring, additive, or packaging migrant. You can select one of these three options by clicking on the appropriate image above the desired assessment type.

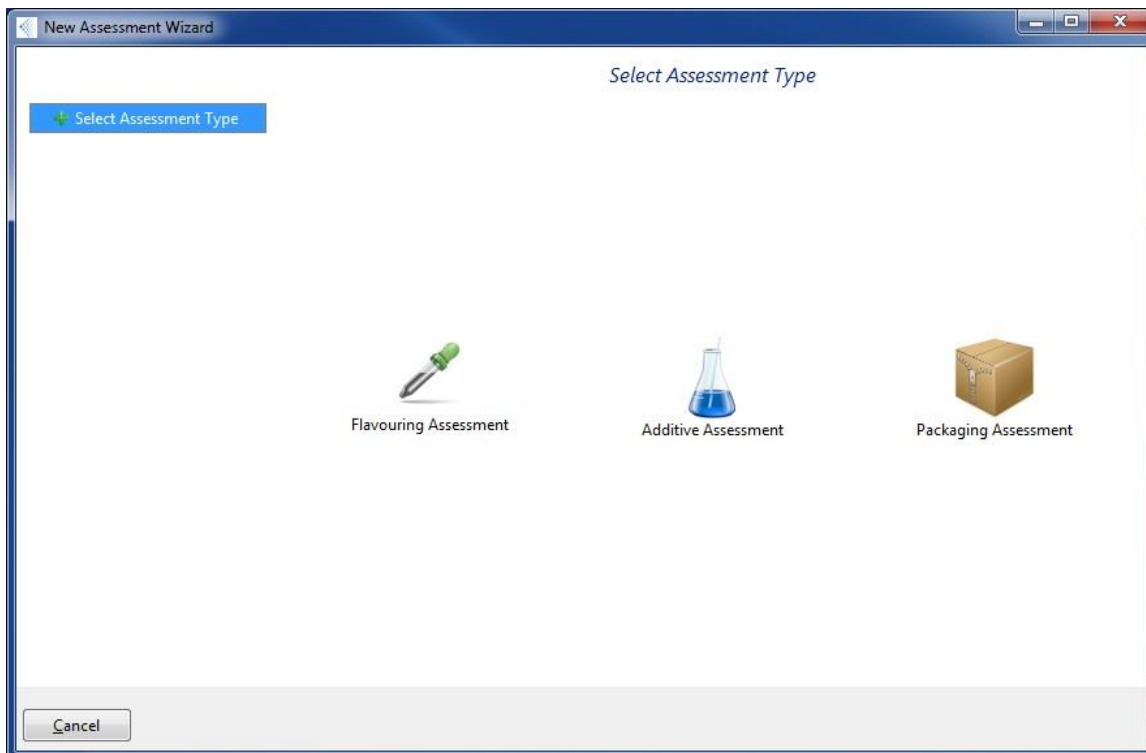


Figure 18: Selecting an assessment type

Select Substance

The target substance for the assessment can be chosen from the list of built-in substances displayed at this step. By default, the option "Use pre-installed FACET data" is selected:

- Use pre-installed FACET data.

This is simply done by clicking anywhere on the row containing the substance of interest, or on the radio button next to the substance ID.

The list of substances may also be searched to find the substance of interest. This search procedure is explained in detail below for each assessment type.

Alternatively, you can use your own table of concentration data to use in an assessment, by selecting the “Use my concentration data” option:

Use my concentration data

This involves populating your own table of concentrations beforehand. See “New Table Wizard” in the “My Data” section of the manual for more details on how to do this.

Searching for a Substance

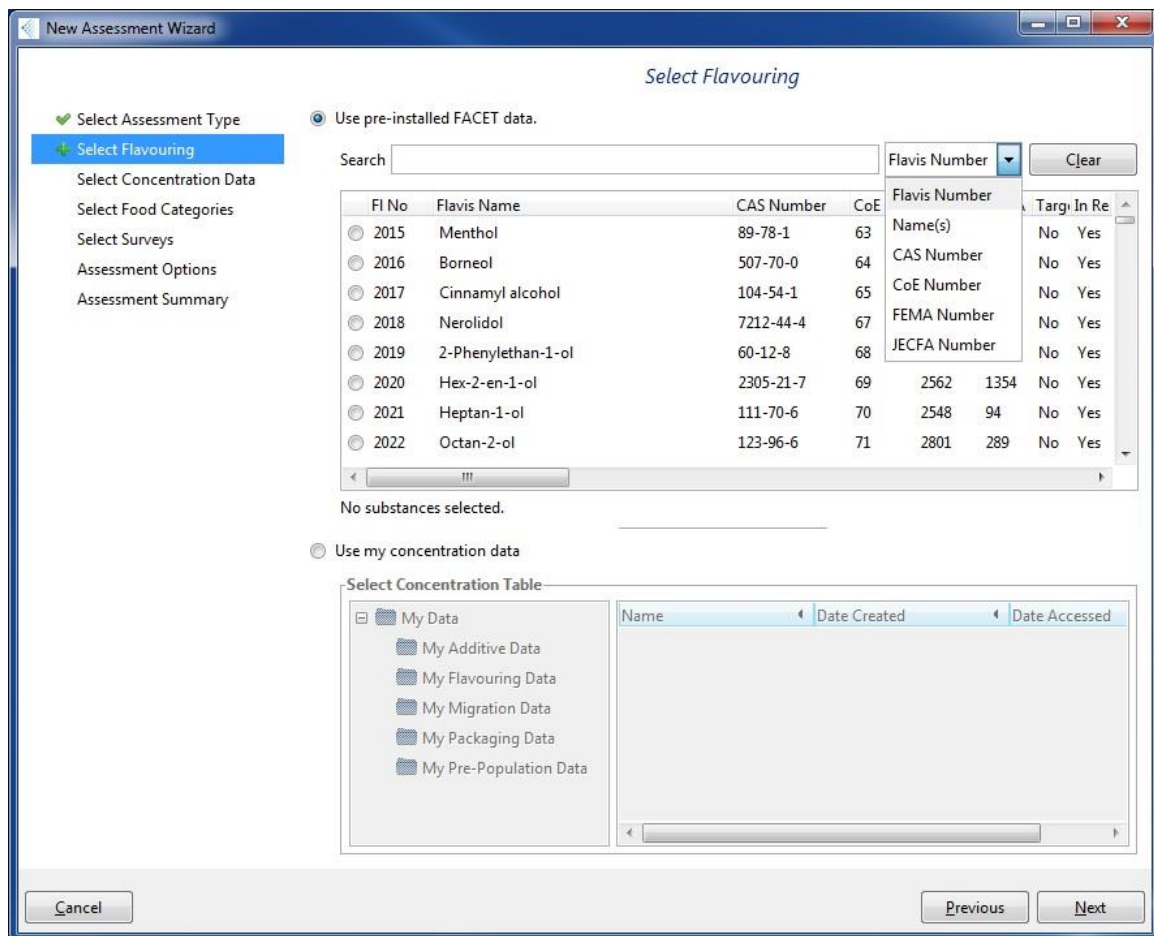


Figure 19: Available search fields for Flavourings

Flavourings

The available search fields for substances assessed as flavourings are Flavis Number, CAS Number, Name(s), CoE Number, FEMA number, and JECFA number. “Instant searching” is enabled in all fields. That is, as you enter search criteria into the search box, search results are returned at each key stroke. A new search can be performed by either deleting what is in the search box or clicking on the “Clear Search” button.

- **Flavis Number:** Numeric field, the number assigned by FLAVIS – the EU Flavour Information System. This is strictly a four or five digit number and is the only unique identifier of flavourings in the FACET project.
- **CAS Number:** This is strictly of the form [up to 7 digits]-[2 digits]-[1 digit], e.g. “64-17-5”, or “0000064-17-5”.
- **Name(s):** This searches both the Flavis Name and Alternative Name fields.
- **CoE Number:** *Council of Europe Number*. This is strictly a numeric field, but can be any length.
- **FEMA Number:** Flavour and Extract Manufacturers Association. This is strictly a numeric field, but can be any length.
- **JECFA Number:** Joint FAO/WHO Expert Committee on Food Additives. This is strictly a numeric field, but can be any length.

Additives

The available search fields for substances assessed as additives are E Number and Name(s). “Instant searching” is enabled in both fields. That is, as you enter search criteria into the search box, search results are returned at each key stroke. A new search can be performed by either deleting what is in the search box or clicking on the “Clear Search” button. The displayed table also indicates whether or not an MPL value is available for that additive.

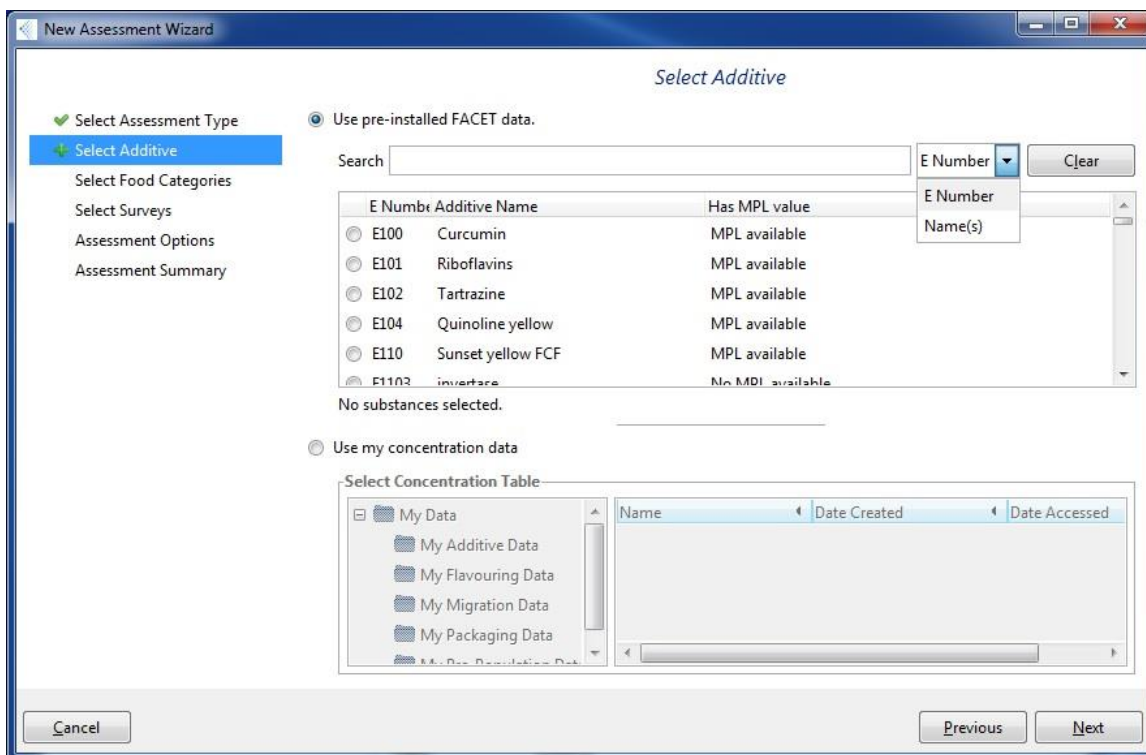


Figure 20: Available search fields for Additives

- **E Number:** This field takes a combination of numbers and letters.
- **Name(s):** This searches the additive name field.

Packaging Migrant

Note that only substances that have been pre-populated using the migration model will appear here. The available search fields for substances assessed as packaging migrants are FACET ID, CAS Number, Name(s), Molecular Formula, and Molecular Weight. The CAS Number field has the same options as those available when searching for flavourings, as described above. “Instant searching” is enabled in all fields. That is, as you enter search criteria into the search box, search results are returned at each key stroke. A new search can be performed by either deleting what is in the search box or clicking on the “Clear Search” button.

- **FACET ID:** This is strictly a four digit number with no leading zeros, e.g. “1021”.
- **CAS Number:** This is strictly of the form [up to 7 digits]-[2 digits]-[1 digit], e.g. “64-17-5”, or “000064-17-5”.

- **Name(s)**: This searches both the Chemical Name and Alternative Name fields.
- **Molecular Formula**: This field takes a combination of letters and numbers.
- **Molecular Weight**: This is strictly a number, with up to a maximum of 3 decimal places, e.g. “60”, “301.5”, “72.345”.
- **Pre-populated**: For each pre-populated substance this field is set to WITHOUT, WITH or BOTH. The first option, WITHOUT, means that the substance was pre-populated without set-off. In the second case, WITH means that the substance was pre-populated with set-off. The third option, BOTH, signifies that the substance was pre-populated both with and without set-off.

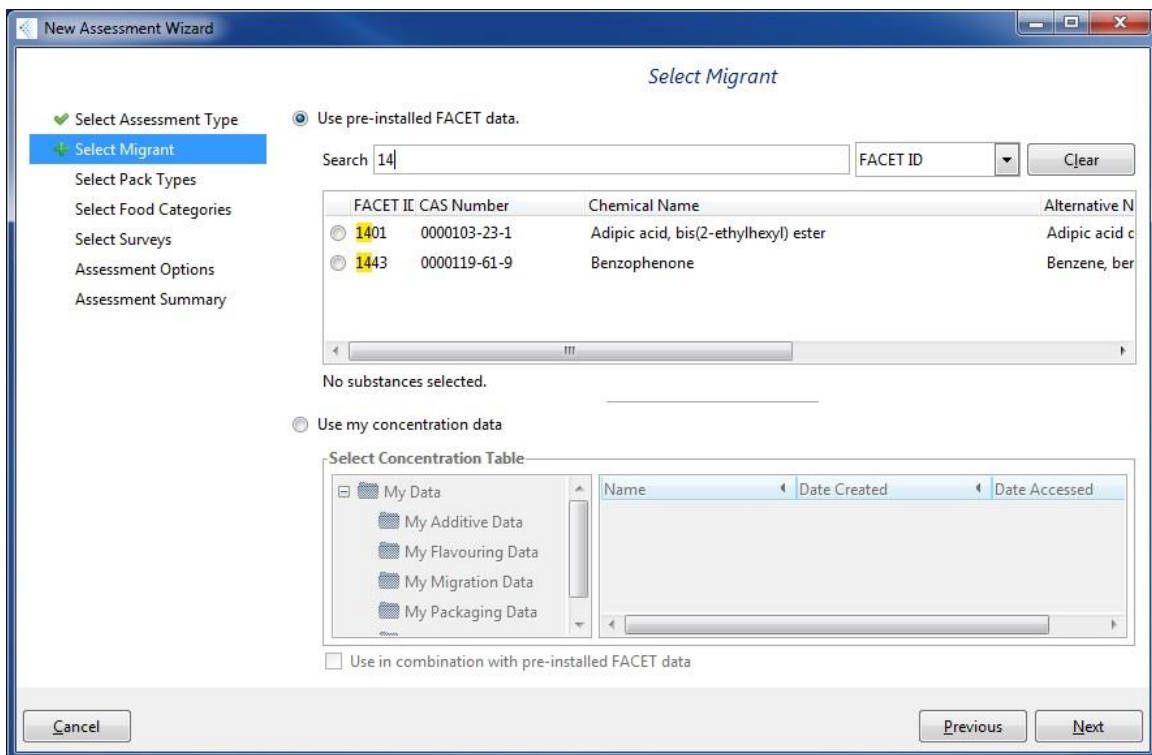


Figure 21: Searching for packaging substances.

Search Results

The search results are returned instantaneously after each keystroke. Once you find the substance you are looking for, select it from the list and click on the “Next” button.

Using Custom Concentration Data

If you want to use a table of pre-loaded concentration data, select this option. The folders in the My Data tab will be made visible and their contents displayed. Select the table you want to use and click “Next”.

The substance used will be unique to the table created. Any food categories created in the table will appear as options in the next step of the wizard, so not all food categories in the table need be used in an assessment.

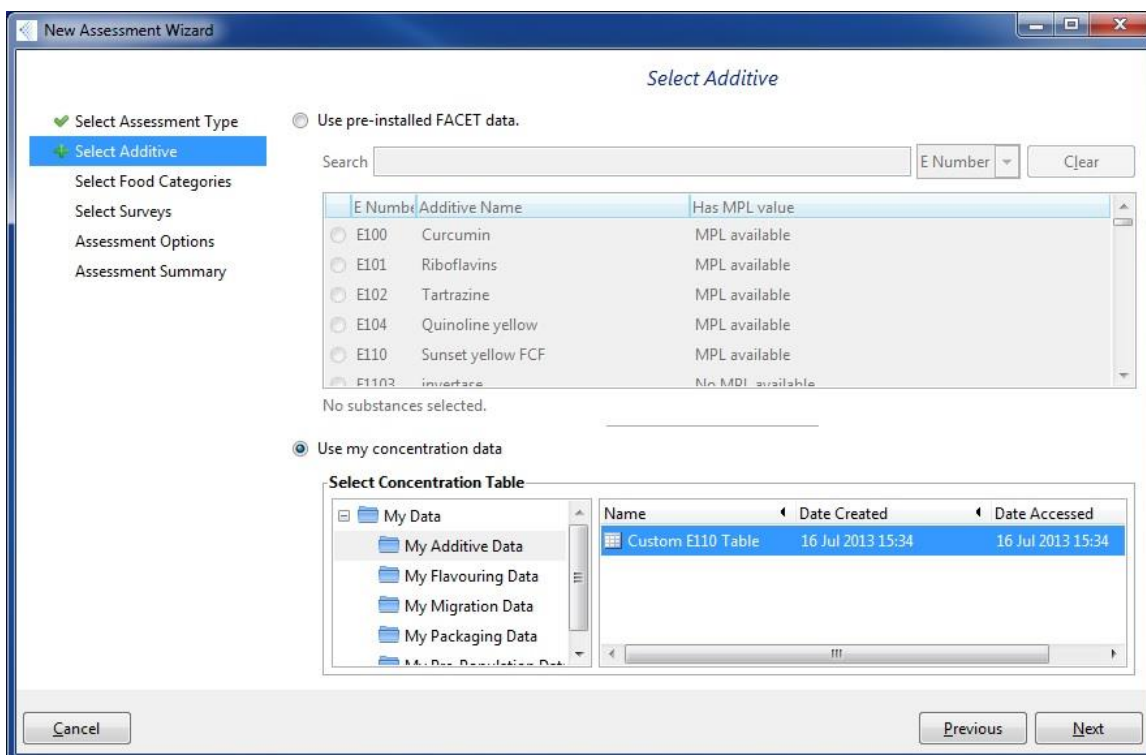


Figure 22: Using custom concentration data

Select Concentration Data

If the substance of interest is a flavouring, the FACET data is divided into eight options:

- Council of Europe, 2000
- EFA (use levels provided to EFSA)
- FEMA (reported in Fenaroli’s Handbook 2005)
- Young et al., 2006
- IOFI JECFA 2006 (use levels provided to JECFA)
- IOFI JECFA 2007 (use levels provided to JECFA)
- IOFI DG SANCO 2007 (use levels provided to JECFA)
- IOFI JECFA 2010 (use levels provided to FACET)

Each dataset has a set of warnings associated with it that the user should consider before performing an exposure assessment with that particular dataset.

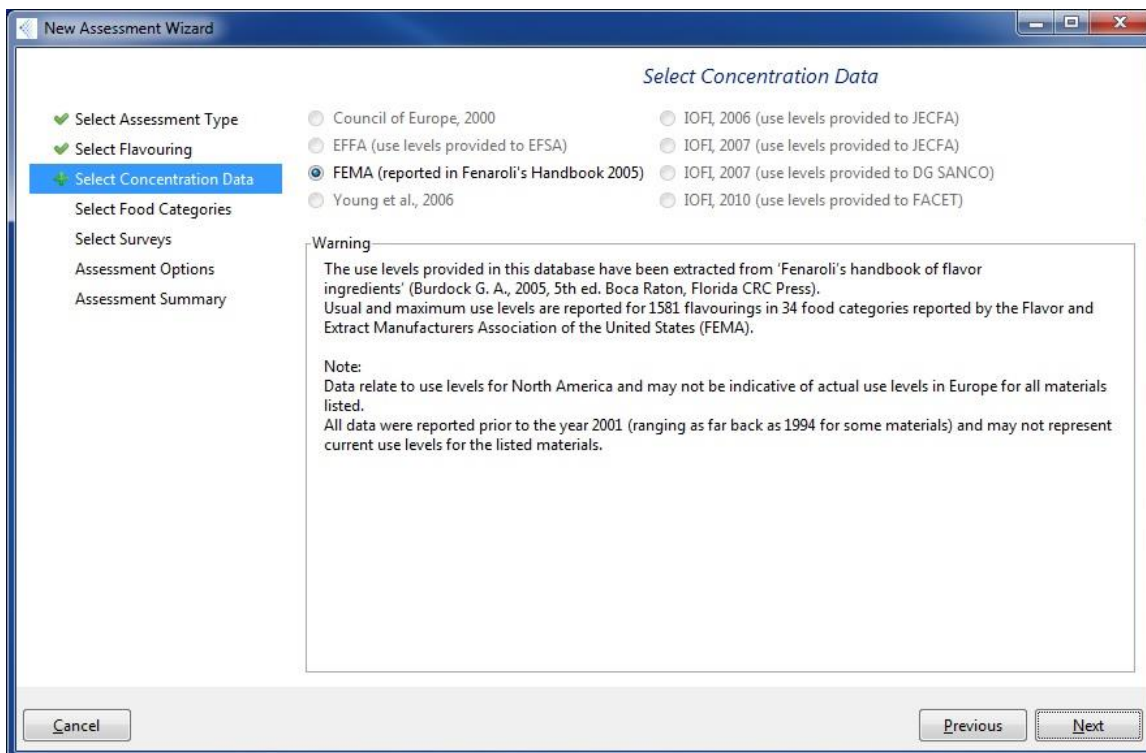


Figure 23: Selecting the source of concentration data

Select Pack Types

If the substance of interest is a packaging migrant, you can select all packaging types or specify which particular types to perform the assessment with. If the substance is a flavouring or additive, this step is skipped.

By default, no pack types are selected for this step. You can select/deselect all packs by clicking on the checkbox at the top left hand corner of this step. The pack types are arranged into four groups; "Main", "Closure", "Outer" and "Insert". To view the contents of a particular pack type, simply click on the plus symbol to the left of that pack type. When pack category is selected, all entries in the tier below are automatically selected too. Tri-state checkboxes are also enabled, whereby a square is shown in the checkbox to indicate the box is neither checked nor unchecked. This is the case when some, but not all, elements of a particular category are checked.

Instant searching is enabled for the pack types. That is, as you enter search criteria into the search box, search results are returned at each key stroke. Sections that match the search are returned highlighted in yellow. To search and select multiple pack types, you can simply search, select packs of interest, and search again. The pack types you selected will remain selected even if they are not displayed.

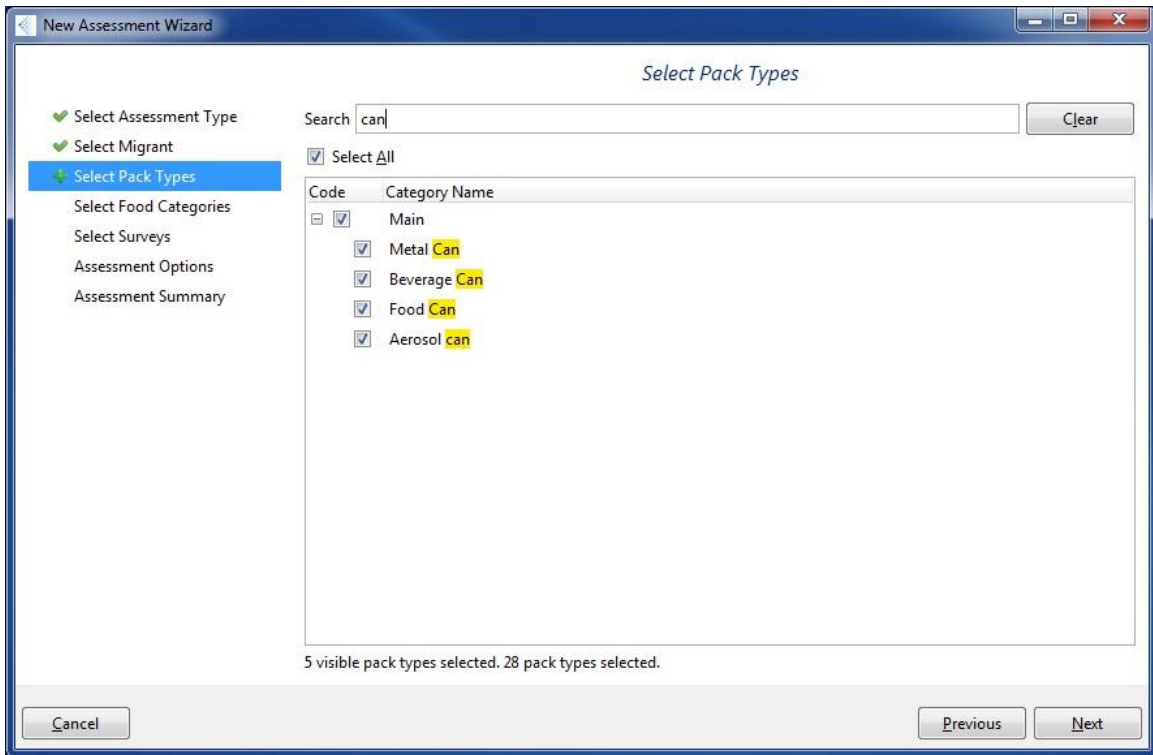


Figure 24: Searching for and selecting pack types.

Food Categories

Here you can select all food categories or specify which food categories you want to perform the assessment with.

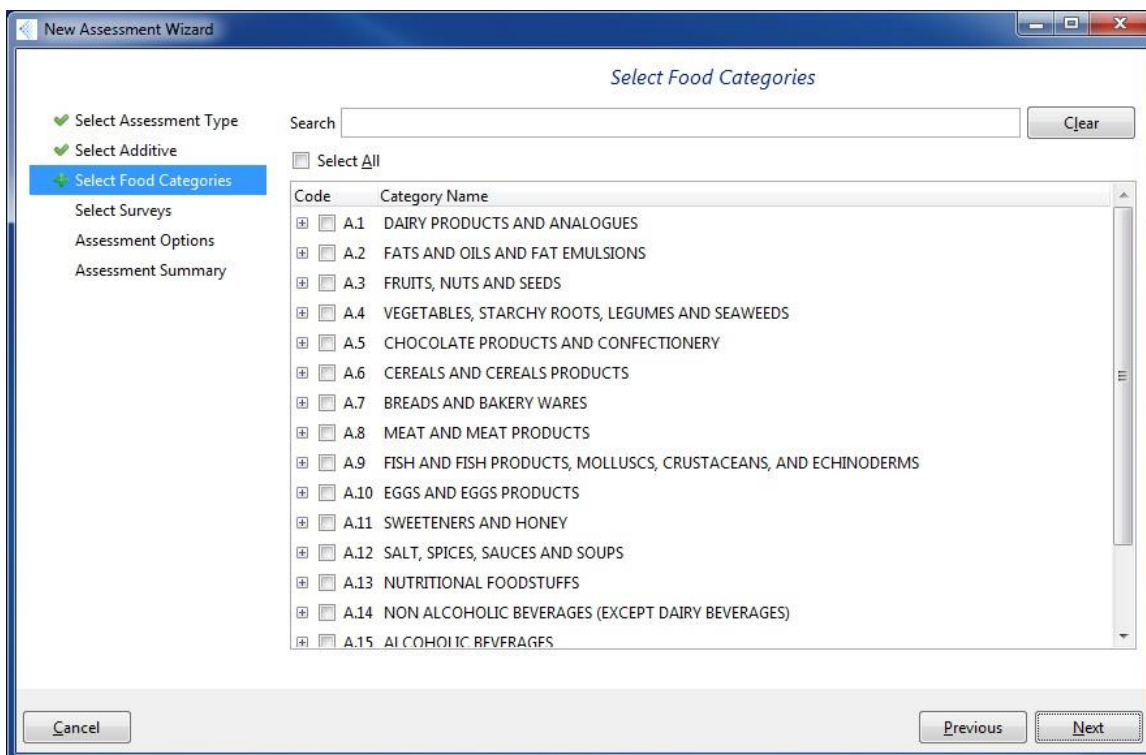


Figure 25: Select Food Categories

By default, no food categories are selected at this step. For all substances, you will be able to explore the relevant food groups, which are divided into 18 top level categories. The letter at the beginning of each food category indicates the type of substance being assessed (“A” for Additive, “F” for Flavouring, “P” for Packaging Migrant).

You can select/deselect all categories by clicking on the “Select All” checkbox at the top right hand corner of the view. To move to a lower tier of a particular food category, simply click on the plus to the left of that category. If there are further tiers within that category, you can click on these to expand them further.

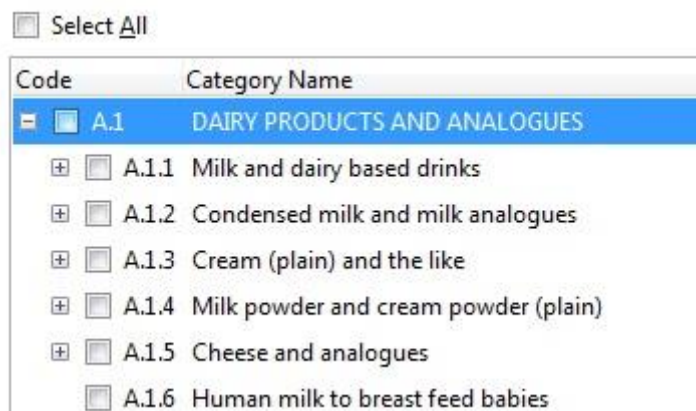


Figure 26: Select all box and expanded tier.

Code	Category Name
<input checked="" type="checkbox"/> A.1	DAIRY PRODUCTS AND ANALOGUES
<input checked="" type="checkbox"/> A.1.1	Milk and dairy based drinks
<input checked="" type="checkbox"/> A.1.1.1	Milk (plain)
<input type="checkbox"/> A.1.1.2	Buttermilk (plain)
<input type="checkbox"/> A.1.1.3	Dairy-based drinks
<input type="checkbox"/> A.1.2	Condensed milk and milk analogues
<input type="checkbox"/> A.1.3	Cream (plain) and the like
<input type="checkbox"/> A.1.4	Milk powder and cream powder (plain)

Figure 27: Further expanded tier and example of tri-state check box.

When a tier is selected, all entries in that tier below are automatically selected too. Tri-state checkboxes are also enabled, whereby a square is shown in the checkbox to indicate the box is neither checked nor unchecked. This is the case when some, but not all, elements of a particular category are checked.

Instant searching is enabled for the food groups. That is, as you enter search criteria into the search box, search results are returned at each key stroke. Sections that match the search are returned highlighted in yellow. To search and select multiple foods, you can simply search, select foods of interest, and search again. The foods you selected will remain selected even if they are not displayed.

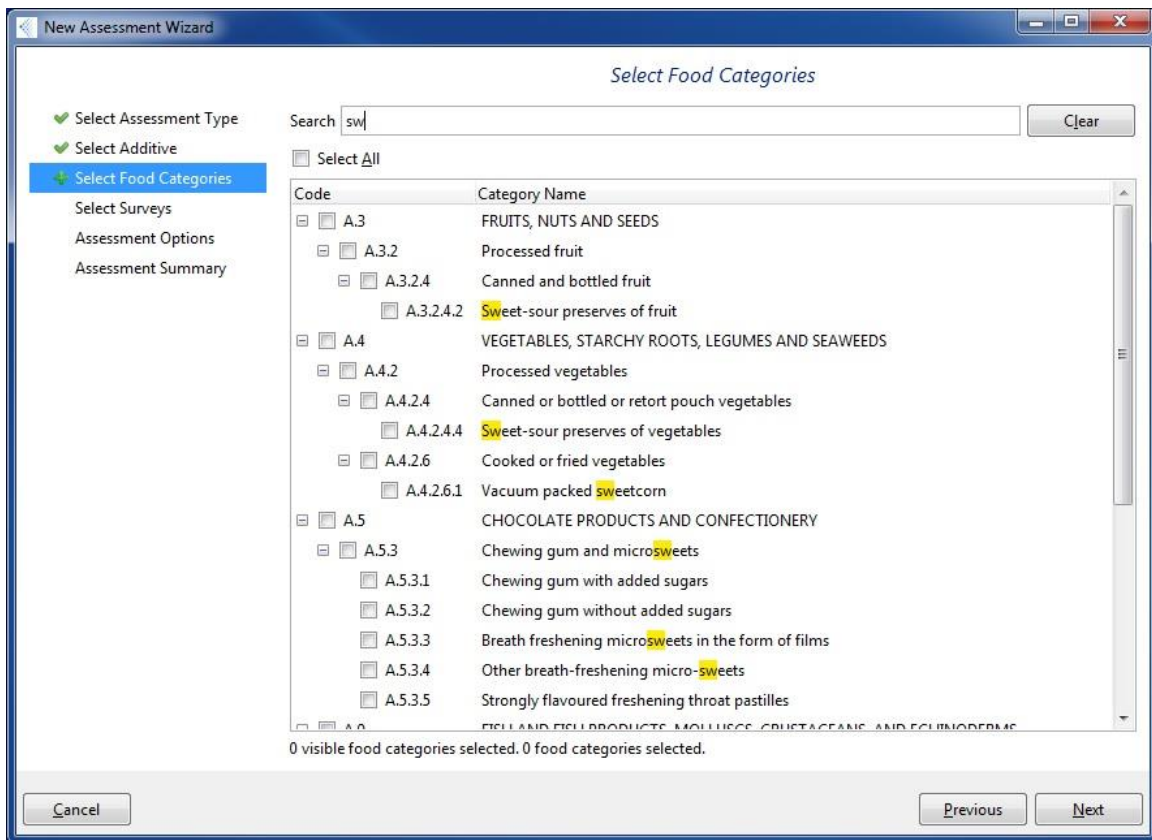


Figure 28: Results returned by each key stroke.

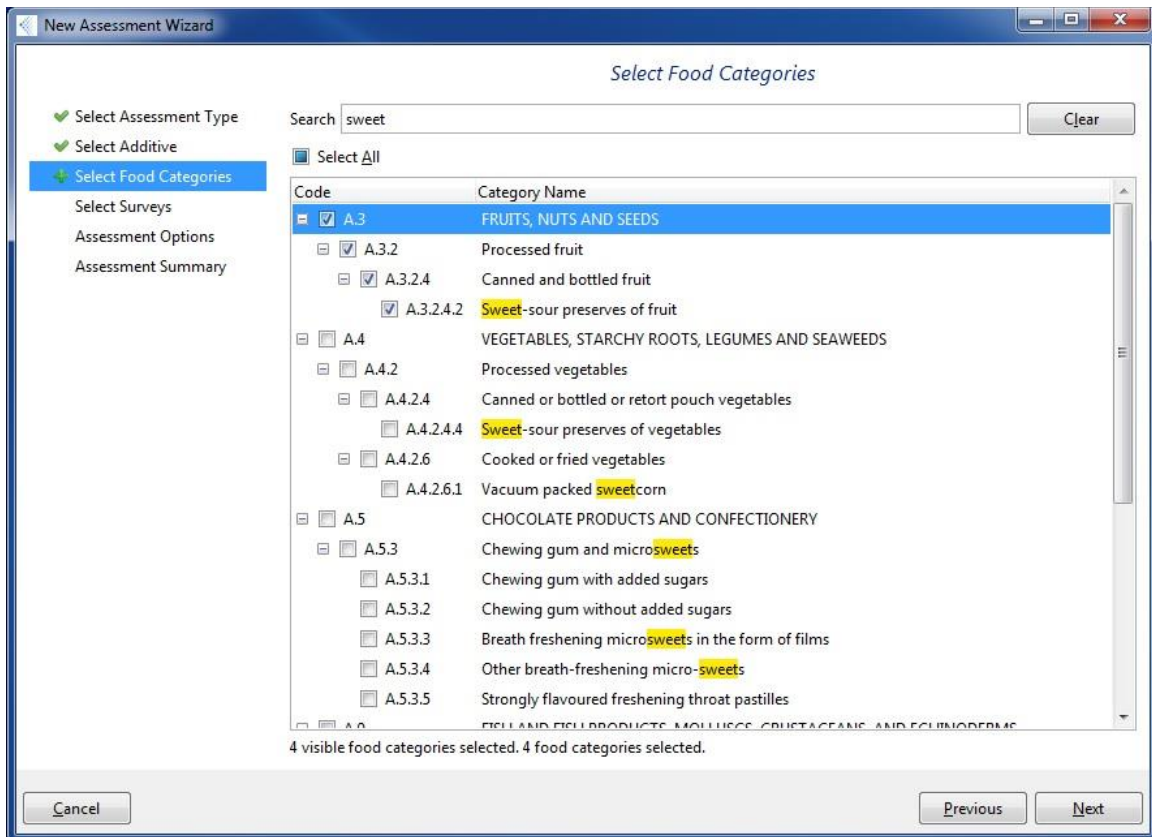


Figure 29: Searching for and selecting food categories

Select Survey

Here, you have the option of using a specific food consumption surveys with which to perform your assessment.

To choose a survey, simply click on your choice from the list and click on the “Next” button. Note that some countries have more than one survey. Multiple surveys can also be selected, and all surveys can be selected for use in an assessment by clicking the “Select All” checkbox in the top left hand corner of the view. Note that selecting all surveys for a particular assessment can take a long time to run.

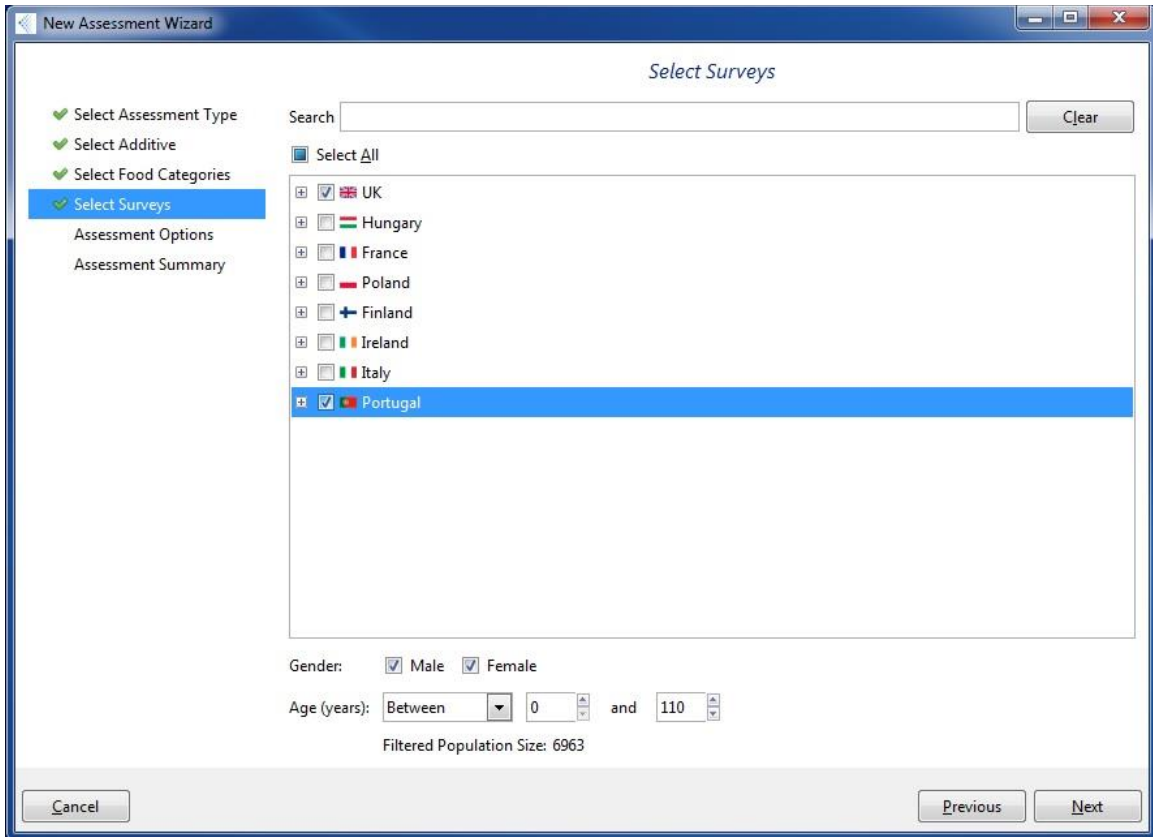


Figure 30: Selecting a survey

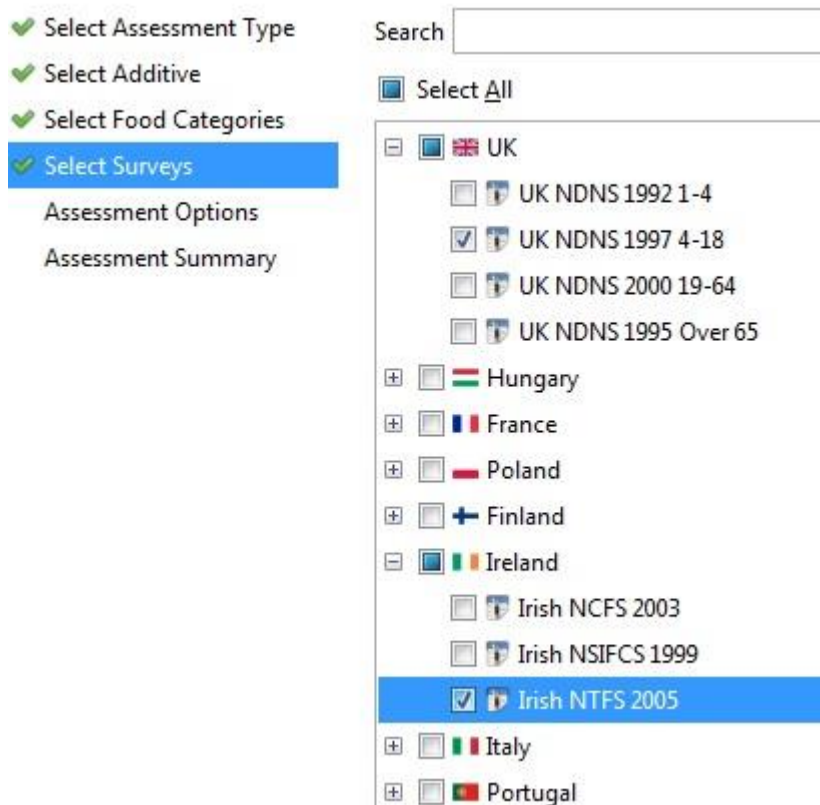


Figure 31: Example of country with multiple surveys and selecting two surveys to compare.

Select Population Filters

Here, you also have the option of using gender and age population filters for your assessment. Selecting one or more of these filters allows you to perform an assessment on that subset of the population. For gender, you can specify whether the subjects of interest are male, female, or both. The “All” option is selected by default. For age, you have the following options from the drop down menu:

- Between (specifying upper and lower limits, inclusively)
- Less than
- Greater than

The user can then enter numeric values relating to the filter chosen from the above list.



Figure 32: Selecting population filters

Note that for an assessment involving multiple surveys, the age filters are applied across all surveys simultaneously, so some age bands may not apply to a given survey.

Assessment Options

In the basic view, you are given the option of naming your assessment and providing a description of the assessment. You can name your assessment and choose a location for it in the Assessments tab by clicking on the “Choose” button. It is recommended that you choose a sufficiently descriptive name other than the default “New Assessment”. In the “Assessment description” text box, the user can enter additional details about their assessment.

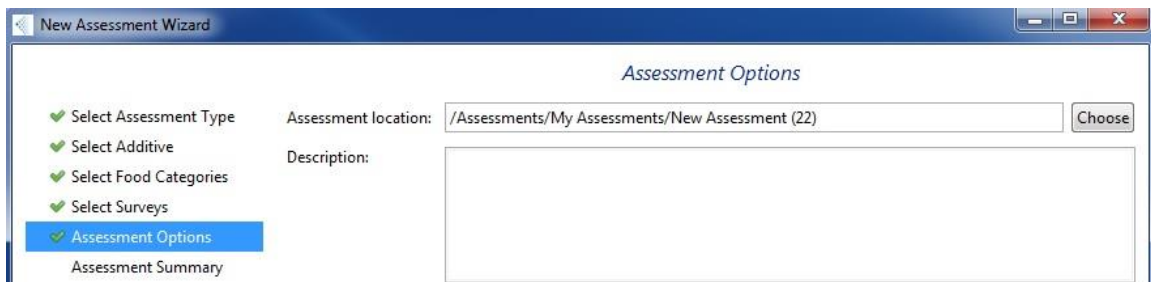


Figure 33: Basic view of assessment options.

You will also need to choose an output folder for your assessment by clicking on the “Choose” button. This opens a pop up window, giving you the option of selecting a destination folder. By default, all assessments are contained in the “Assessments” folder. You can create a subfolder by clicking on the “New Folder” button at the bottom of the dialogue box, and then entering a name for the new folder. Alternatively, right click on where you want to create the folder and select “New Folder” from the context menu.

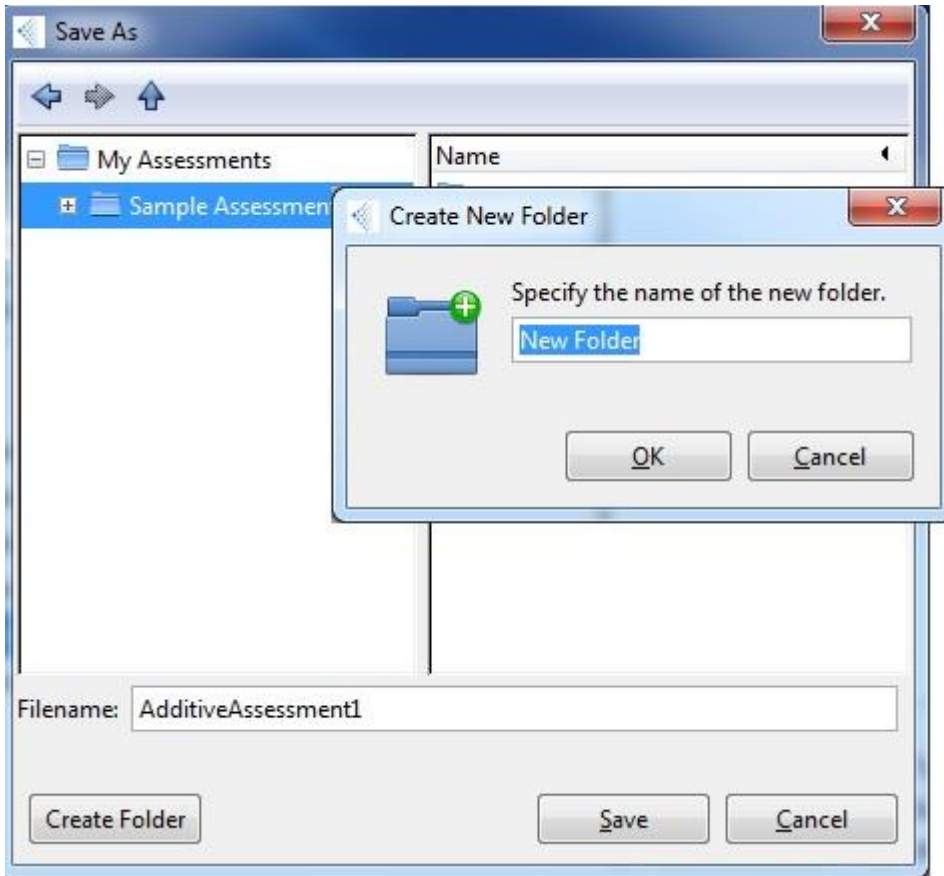


Figure 34: Choosing an output folder.

Flavouring Assessment Options

Depending on the substance and database chosen, you have a number of options for a flavouring assessment:

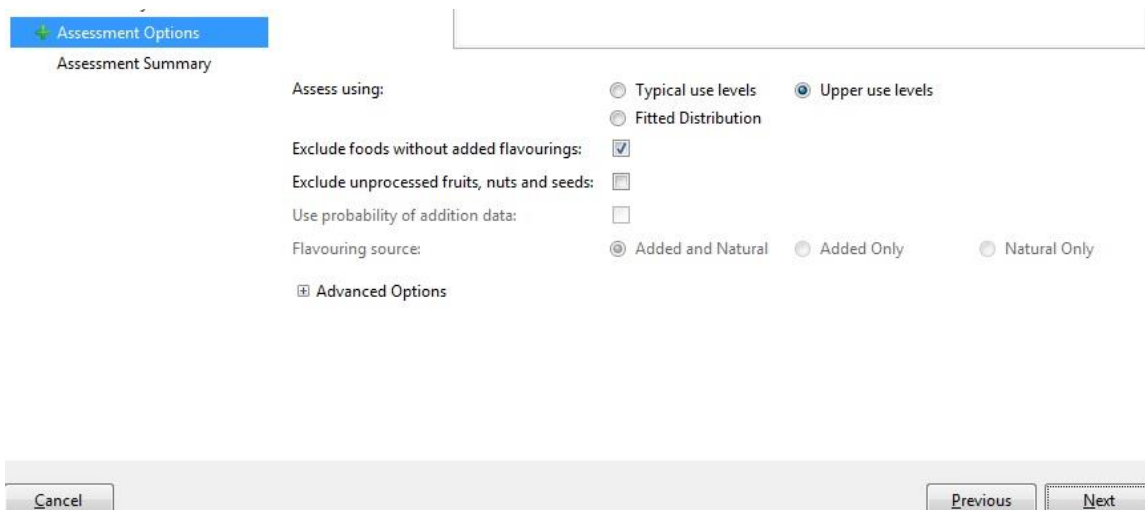


Figure 35: Flavouring options

Assess using: The exposure assessment can be performed using either:

- Typical use levels
- Upper use levels
- Fitted distribution (a parametric distribution fitted to the typical and upper use levels)

Exclude unflavoured foods: Consumption events described as being “without added flavourings” are ignored in the exposure assessment.

Exclude homemade foods: Consumption events described as being homemade are ignored in the exposure assessment.

Use probability of addition data: Use probability of addition data for flavourings that have this value assigned (only applies to the target flavourings in FACET).

Flavouring source: Assess exposure due to:

- Added and natural
- Added only
- Natural only

The option for assessing exposure due to natural occurrence only applies to the target flavourings in FACET.

Additive Assessment Options

Depending on the substance chosen, the user has a number of options for an additive assessment:

Assessment Options
Assessment Summary

Assess using:

- Typical Minimum
- Typical Maximum
- Extreme Minimum
- Extreme Maximum
- Fitted Distribution
- MPL

Include occurrence data:

Advanced Options

Cancel Previous Next

Figure 36: Additive options.

Assess using: The exposure assessment can be performed using:

- Typical minimum concentrations
- Typical maximum concentrations
- Extreme minimum concentrations
- Extreme maximum concentrations
- Fitted distribution
- Maximum Permitted Levels (MPLs)

The first five options only apply to the 32 target additives and are based on data supplied by industry.

Packaging Assessment Options

Consumer loyalty: For a packaging assessment, you can choose to perform the assessment with, without, or both with and without consumer loyalty model (this appears in the advanced options for the other assessment types).

SetOff: If the substance in the assessment has been pre-populated with set-off then, at this point, the user has the option to run the assessment with set-off. Otherwise, the user will not be allowed to check the “Use SetOff” option.

Exclude homegrown/homemade foods: Consumption events described as involving homegrown foods are ignored.

Exclude restaurant/canteen foods: Consumption events described as involving restaurant or canteen foods are ignored.

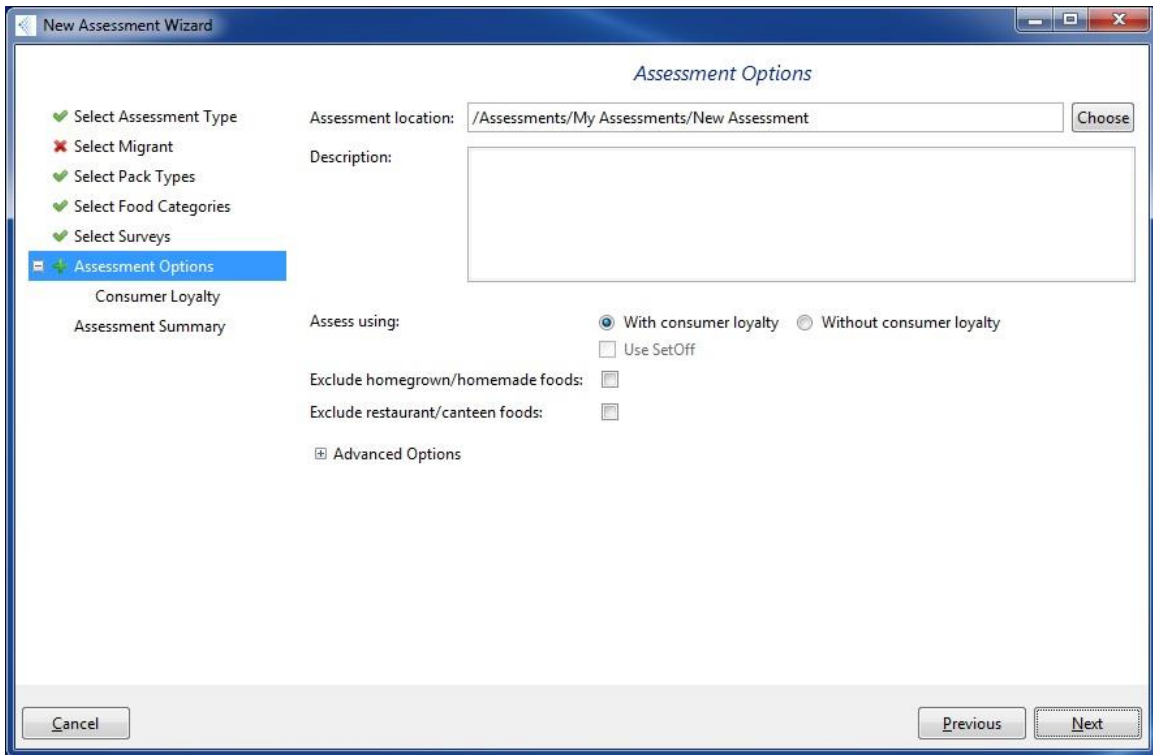


Figure 37: Assessment Options

Advanced Options

If the “Show Advanced Options” option is clicked, you are presented with additional options relating to the statistics of the assessment.

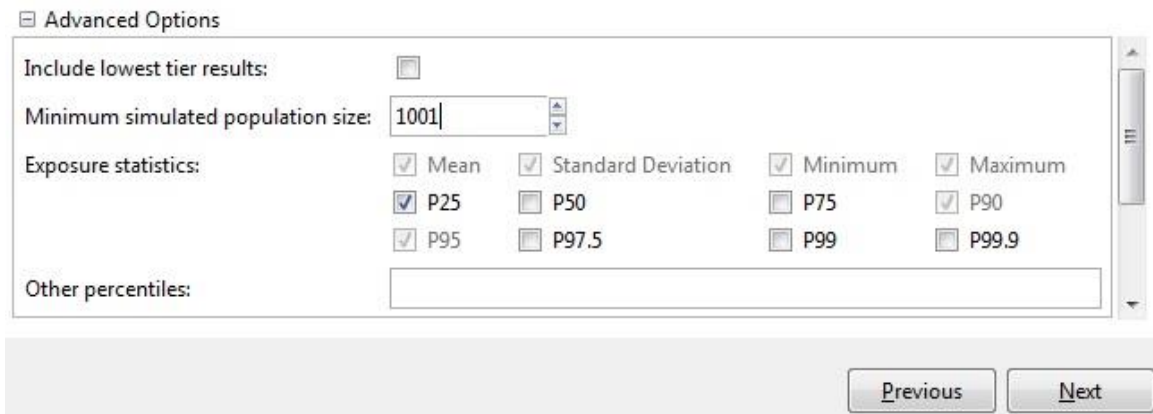


Figure 38: Advanced Options

These are:

- **Include lowest tier results:** Include output for all food categories at the lowest tier. Note that this causes the assessment to take much longer to run.

- **Minimum simulated Population Size:** This is a numeric field, allows the user to change the size of the population used in the simulation. The number specified is the minimum population size used in the assessment; the actual number used will be increased to the next multiple of the number of subjects chosen after the filtering in Step 7.
- **Exposure Statistics:** These are checkboxes that allow the user to include the following statistics in the assessment (the first four options, P90, and P97.5 are selected by default):
 - Mean
 - Standard Deviation
 - Minimum
 - Maximum
 - P25
 - P50
 - P75
 - P90
 - P95
 - P97.5
 - P99
 - P99.9
- **Other Percentiles:** This is a numeric field. Other percentiles can be entered, separated by commas (e.g. 92, 93).
- **Confidence Intervals:** These are checkboxes that allow the user to specify the following confidence intervals (the standard error is selected by default):
 - Standard Error
 - 90% Confidence Interval
 - 95% Confidence Interval
 - 99% Confidence Interval
- **Other Confidence Intervals:** This is a numeric field. Other confidence intervals can be entered, separated by commas (e.g. 75, 85).
- **Use consumer loyalty:** For additives and flavourings, a consumer loyalty model can be used as part of the exposure assessment. This brings up a new set of food categories to used in the consumer loyalty model.
- **Truncate at SML value:** This only applies to packaging assessments. If chosen, an SML can be entered to truncate concentration values calculated by the migration model.

Assessment Summary

This step presents you with a summary of the current choices of substances, populations and food categories for the assessment.

After reviewing the choices, you can choose to start an assessment using the “Run” button at the bottom right of the window. At the bottom of the summary the estimated time for the assessment to run is shown. In order to start the assessment you must first check the box indicating that you understand that your computer will be busy for the time taken to run the assessment.

Equally, you may wish to make changes to the selections. Navigation to the appropriate steps to do this is easily achieved with the buttons on the left of the tab.

FACET Data

The FACET data tab allows you to view (but not edit) FACET data used in performing exposure assessments. Note that raw concentration data, packaging data, and consumption diaries will be hidden from the user at all times.

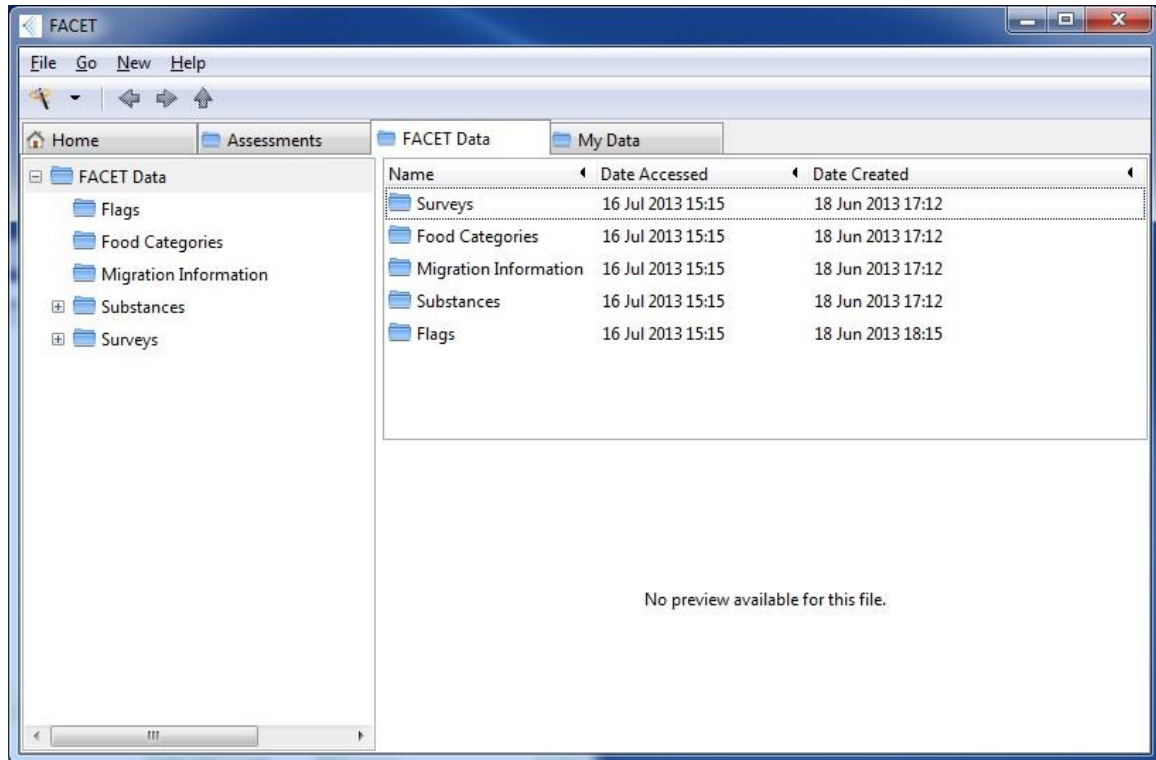


Figure 39: The FACET Data Tab

The tab is implemented in a three pane layout. The upper pane contains folders of data tables that can be selected and viewed, and left-hand pane shows a tree structure that shows how the FACET folders are organised. The bottom pane displays the contents of certain tables in the upper pane.

There are six main folders:

- Flags
- Food Categories
- Migration Information
- Substances
- Surveys

Clicking on the plus symbol next to each folder in the folder tree causes the contents of the tree to expand. Each folder is described in detail below.

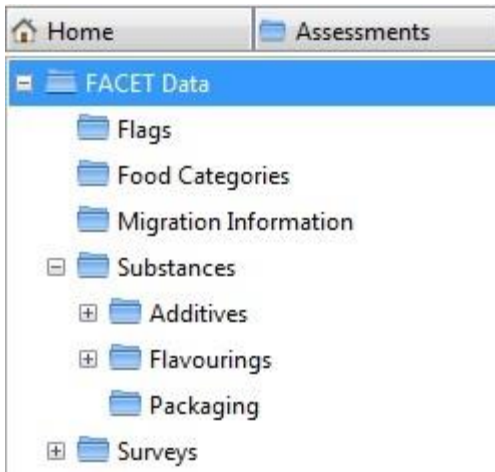


Figure 40: Expanding folders using the plus symbol.

Flags

This folder contains tables of the different possible flags used in the consumption diaries and chemical concentration tables. Flags with the same meaning and settings are grouped in the same tables. Both the numerical value and the text description of the flag settings are given in each table.

Food Categories

This folder provides a list of all food categories in FACET. The food categories are hierarchical, and there is a separate system for flavourings, additives and packaging. There are three systems:

- Additives Food Hierarchy
- Flavourings Food Hierarchy
- Packaging Food Hierarchy

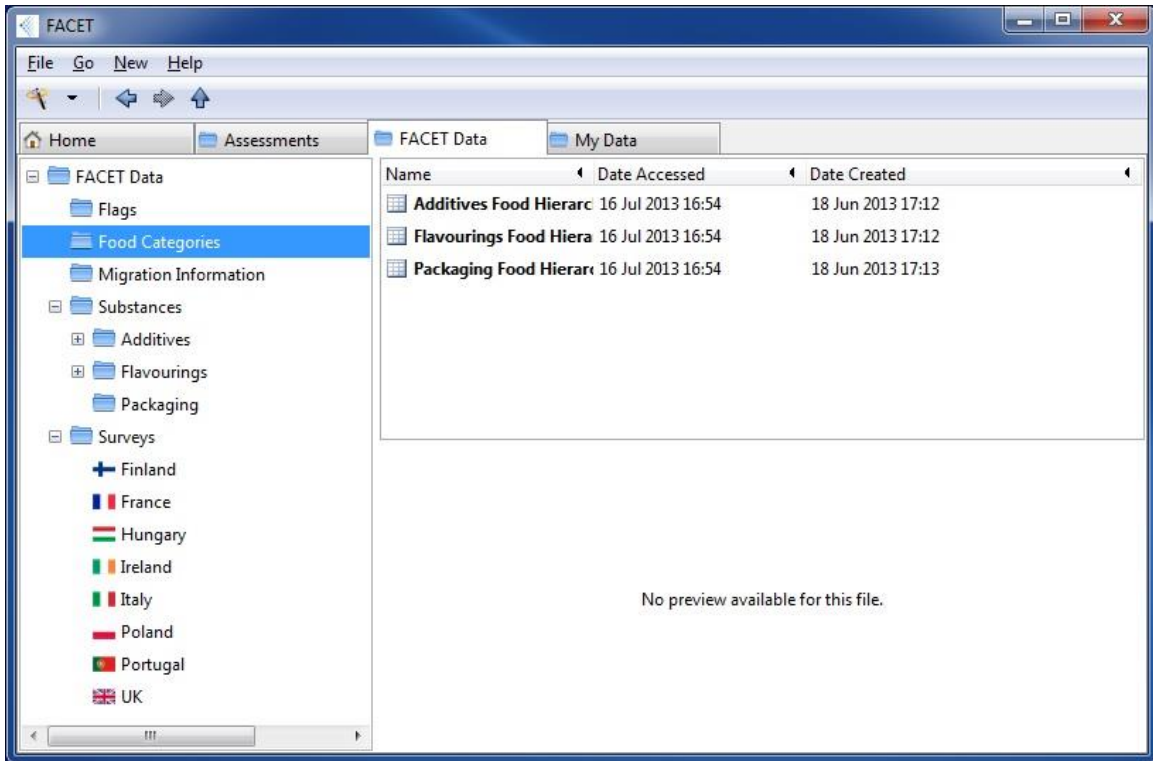


Figure 41: Food Categories Folder.

Clicking on each table causes it to appear in the pane below. The fields in each table are:

- Category Code
- Category Name

The screenshot shows a software interface with two main panes. The top pane displays a table with three columns: Name, Date Accessed, and Date Created. The bottom pane displays a table with two columns: Code and Category Name. A search box with a 'Clear' button is located between the two panes.

Name	Date Accessed	Date Created
Additives Food Hierarc	16 Jul 2013 16:54	18 Jun 2013 17:12
Flavourings Food Hiera	16 Jul 2013 16:54	18 Jun 2013 17:12
Packaging Food Hierarc	16 Jul 2013 16:54	18 Jun 2013 17:13

Code	Category Name
F.1	Dairy products and analogues including ingredients of composite foods
F.2	Fats and oils and fat emulsions including ingredients of composite foods
F.3	Fruits, nuts and seeds including ingredients of composite foods
F.4	Vegetables, starchy roots, legumes and seaweeds including ingredients of composite f...
F.5	Chocolate products and confectionery including ingredients of composite foods
F.6	Cereals and cereal products including ingredients of composite foods
F.7	Breads and bakery wares including ingredients of composite foods
F.8	Meat and meat products including ingredients of composite foods

Figure 42: Fields available in each table.

Each system can be viewed as a tree, and clicking on the arrow in each category causes the contents of that category to be displayed, which in turn can be expanded and so on. You can also search the data using the search box that appears between the panes.

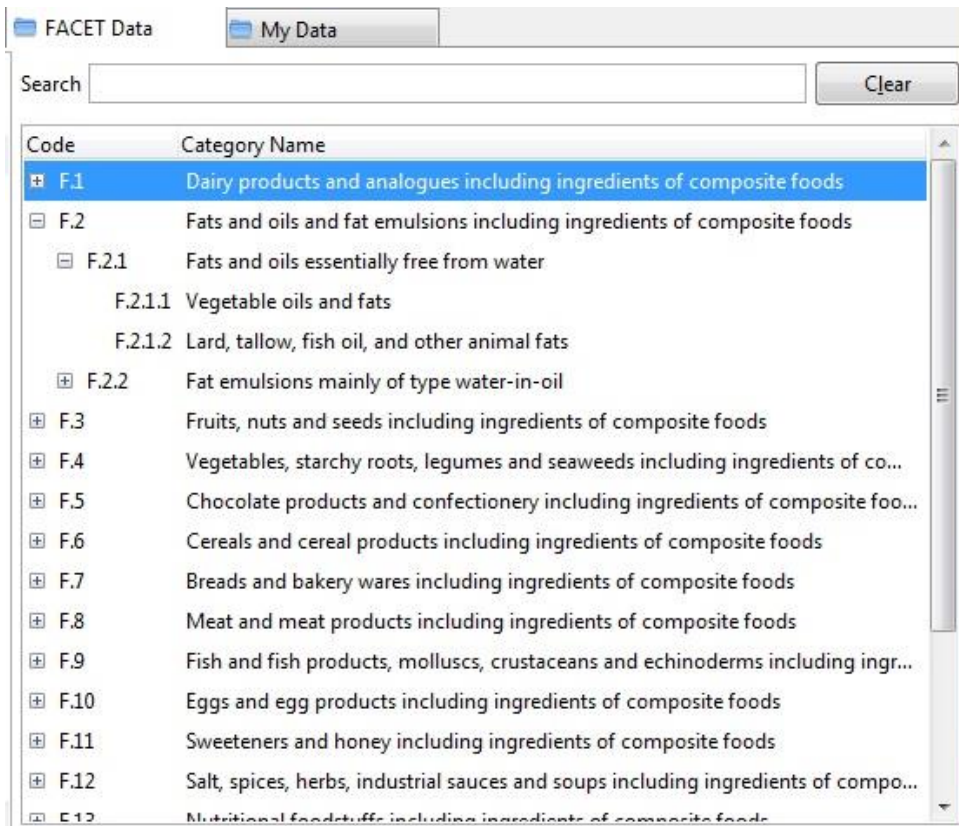


Figure 43: Example of category tree.

Migration Information

This folder contains all material codes and pack types used in FACET.

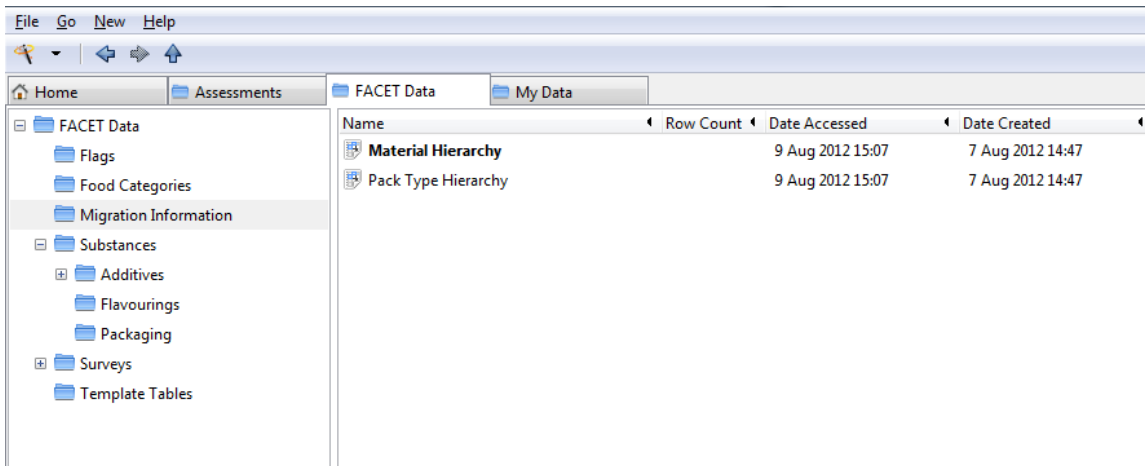


Figure 44: Material Code folder.

The fields in the Material Hierarchy table are:

- Material Code
- Material Name

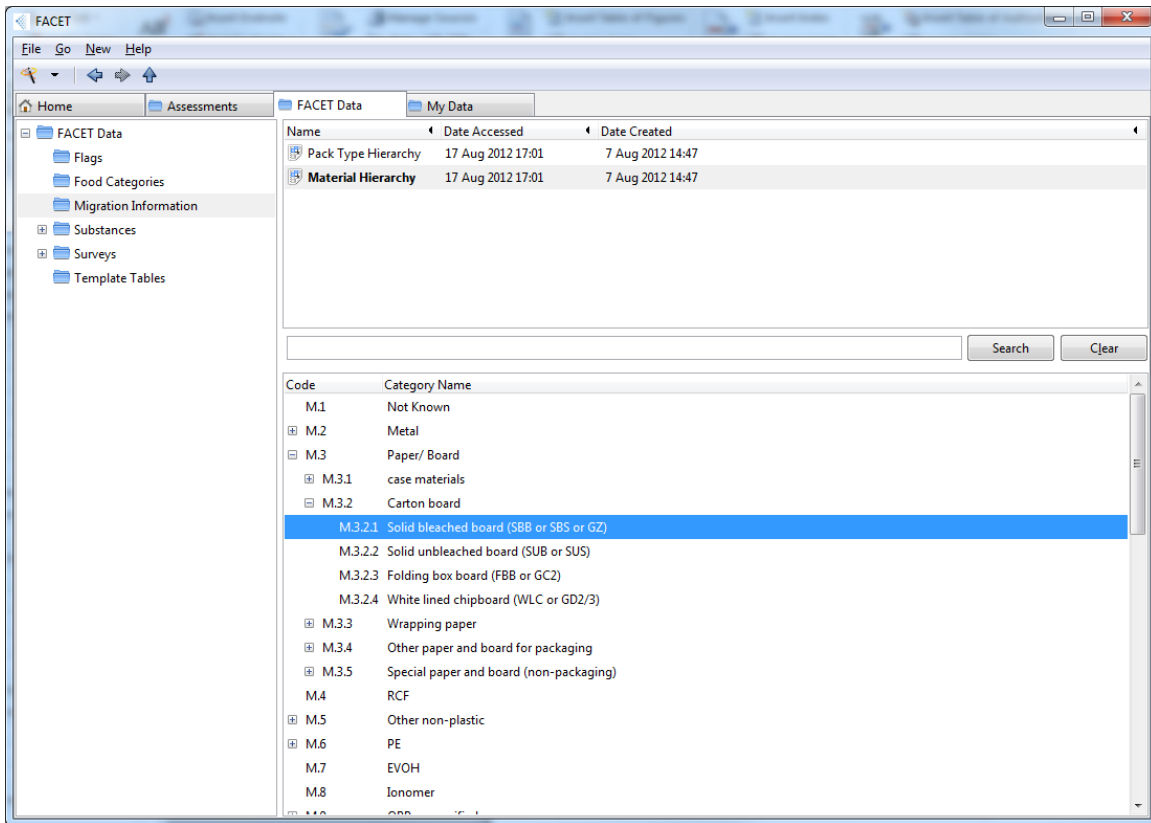


Figure 45: Material Code Table

The material codes can be viewed as a tree, and clicking on the arrow in each category causes the contents of that category to be displayed, which in turn can be displayed. You can also search the data using the search box that appears between the panes.

The Pack Type Hierarchy table shows the pack type descriptions contained in the Main, Closure, Outer, and Insert components of food packaging. It is in a hierarchy in the same form as the Material Hierarchy table.

Substances

This view provides a list of all substances in FACET. There are three folders, each of which is described in detail below. Double-clicking on any of the tables will open a data view of that table for so that the content can be browsed easily.

Name	Date Accessed	Date Created
Additives	Feb 28 09:10	Feb 27 12:37
Flavourings	Feb 28 09:10	Feb 27 12:37
Packaging	Feb 28 09:10	Feb 27 12:37

Figure 46: Substances folders.

Flavourings

The flavourings folder contains tables of all of the flavourings data in FACET. There are two subfolders; the Flavouring Info folder and the Screening Calculations folder.

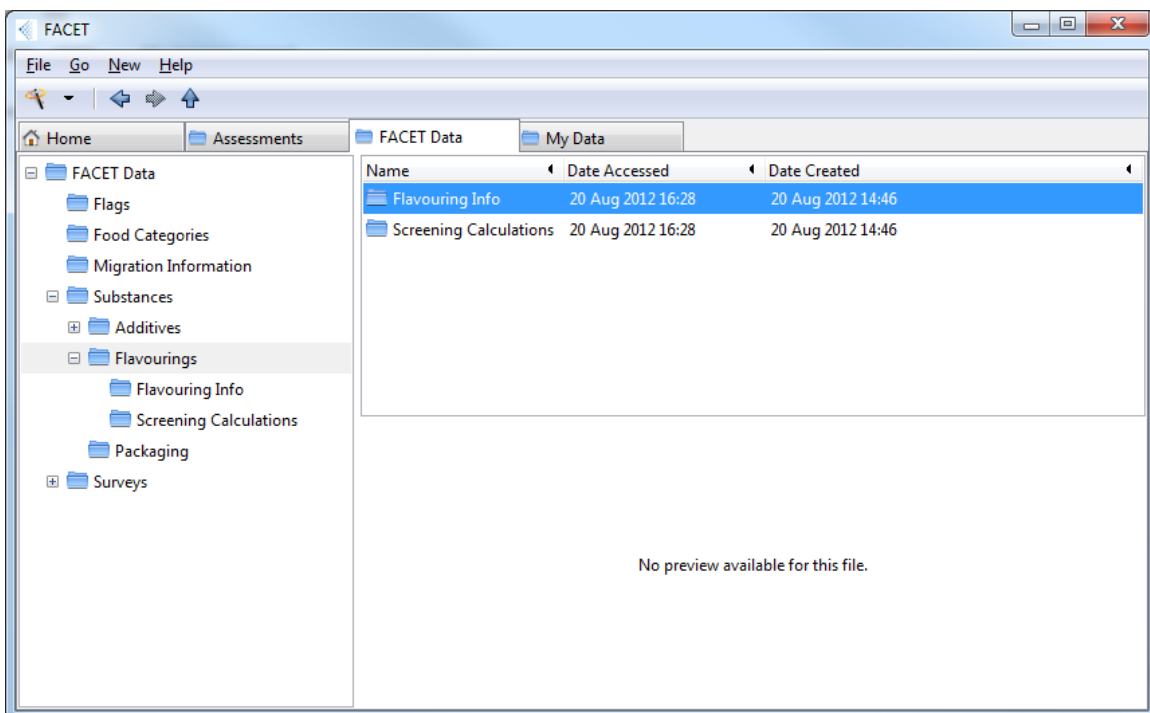


Figure 47: Flavourings folder

Flavourings Info

This folder contains tables detailing all the information on flavouring concentrations and other information.

The flavourings table (simply called “Flavourings”) contains information on all the different flavouring substances in FACET. Clicking on the table once will bring up a preview in the bottom right pane, showing a search box for browsing different fields. The table contains the following fields:

Fl No	Flavis Name	Flavis Number	CoE No	FEMA No	Jecfa N	T
2015	Menthol		63		427	N
2016	Borneol		64	2157	1385	N
2017	Cinnamyl alcohol		65	2294	647	N
2018	Nerolidol		67	2772		N
2019	2-Phenylethan-1-ol		68	2858	987	N
2020	Hex-2-en-1-ol	2305-21-7	69	2562	1354	N

Figure 48: Search options for flavouring data.

- **Flavis Number:** Numeric field, the number assigned by FLAVIS – the EU Flavour Information System.
- **Flavis Name:** The name assigned by FLAVIS – the EU Flavour Information System.
- **CAS Number:** Chemical Abstracts Service. This is strictly of the form [up to 7 digits]-[2 digits]-[1 digit], e.g. “64-17-5”, or “0000064-17-5”.
- **CoE Number:** Council of Europe Number. This is strictly a numeric field, but can be any length.
- **FEMA Number:** Flavour and Extract Manufacturers Association. This is strictly a numeric field, but can be any length.
- **JECFA Number:** Joint FAO/WHO Expert Committee on Food Additives. This is strictly a numeric field, but can be any length.
- **Target Flavouring:** Yes/No field.
- **In Register:** Yes/No field.
- **Evaluation Status:** Whether evaluated or not and by whom.
- **Short Reference:** Reference to when the flavouring was assessed.
- **Synonymous:** Any synonyms for the flavouring.
- **Remarks:** Any further information about the flavouring.

There are 15 other tables in this folder:

- **Flavourings Refined:** The probability of addition of the target flavourings in difference FACET food categories, and refined use levels where known.
- **Flavourings EFA:** Upper and average use levels from the European Flavour Association, in both the FACET and EFA food categories.
- **Flavourings FEMA:** Upper and average use levels from the Flavour and Extract Manufacturers Association, in both the FACET and FEMA food categories.
- **Flavourings IOFI JECFA 2006:** Flavouring concentration database.
- **Flavourings IOFI JECFA 2007:** Flavouring concentration database.
- **Flavourings IOFI JECFA 2010:** Flavouring concentration database.
- **Flavourings IOFI:** Flavouring concentration database.

- **Flavourings DGSanco:** Flavouring concentration database.
- **Flavourings CoE:** Flavouring concentration database.
- **Flavourings Smoke:** Flavouring concentration database.
- **Conversion Factors:** Table of conversion factors for different food combinations.
- **Flavourings Natural Flag Setting:** For a given flag, shows for what foods with that flag setting are used to calculate a concentration value.
- **Flavourings Natural Food Categories:** What food categories can occur as recipe fractions.
- **Flavourings Natural Recipe Data:** What flags can occur as ingredient fractions.
- **Flavourings Natural:** Flavouring concentration database.

The Conversion Factors table can be modified to assess the impact of changing different conversion factors. The field that can be edited is in white. In order to restore the default values, click the “Restore Default” icon in the tool bar.

	Ordine	FACET Code	FACET Description	Default Conversion Factor	Conversion Factor	
1	2	F.1.1	Milk and dairy based drinks	1	1	NULL
2	3	F.1.1.1	Milk (plain)	1	1	NULL
3	4	F.1.1.2	Buttermilk (plain)	1	1	NULL
4	5	F.1.1.3	Dairy-based drinks, flavoured	1	1	NULL
5	7	F.1.2.1	Condensed milk	3	3	NULL
6	8	F.1.2.2	Milk analogues	1	1	NULL
7	9	F.1.2.2.1	Soy and other vegetable	1	1	NULL
8	10	F.1.2.2.2	Beverage whiteners	1	1	NULL
9	11	F.1.2.2.3	Other milk analogues	1	1	NULL
10	12	F.1.3	Cream (plain) and the like	1	1	NULL
11	13	F.1.3.1	Cream (plain) pastourized	1	1	NULL
12	14	F.1.3.2	Cream analogues (including	1	1	NULL
13	15	F.1.4	Milk powder and cream powder	7	7	NULL
14	16	F.1.4.1	Dried milk and dried skim	7	7	NULL
15	17	F.1.4.2	Milk powder for vending machines	7	7	NULL

Figure 49: Conversion Factors Table



Figure 50: Restore Default Icon

Screening Calculations

This folder contains tables of screening calculations for the different databases, namely the APET, SPET, TAMDI, and mTAMDI methods.

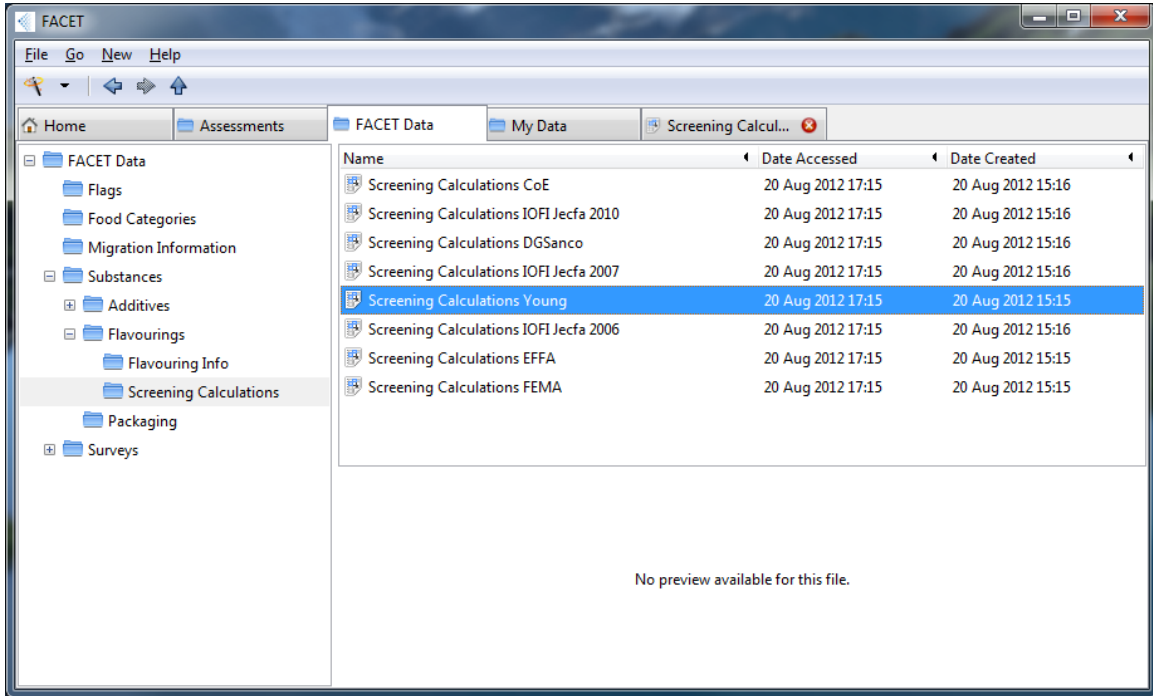


Figure 51: Screening Calculations Folder

Additives

The additive folder contains two subfolders; “Additive Info” and “Additive Ingredient Distributions”.

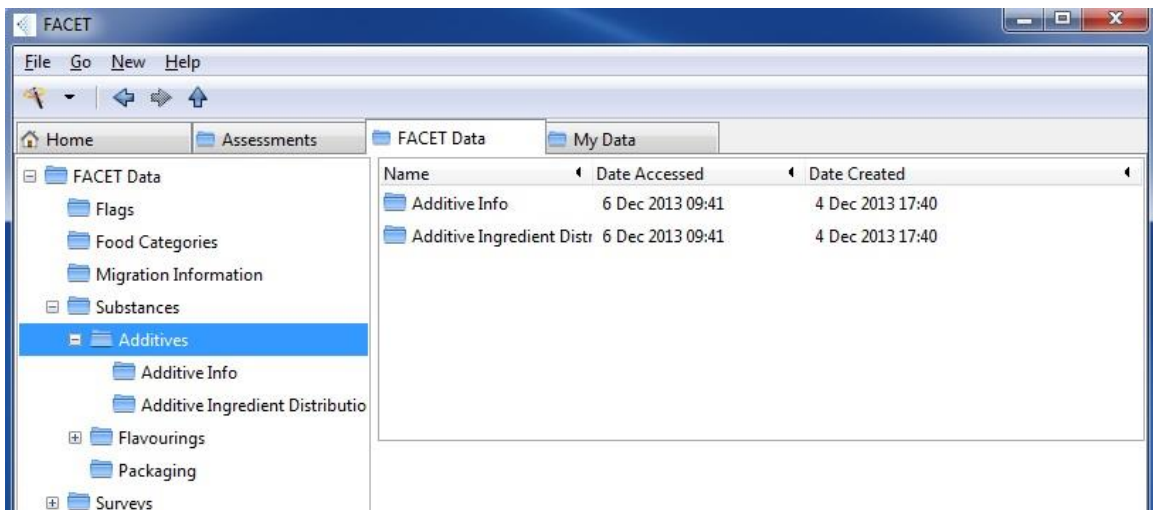


Figure 52: Additive Folder

Additive Info

The additive info folder contains three tables.

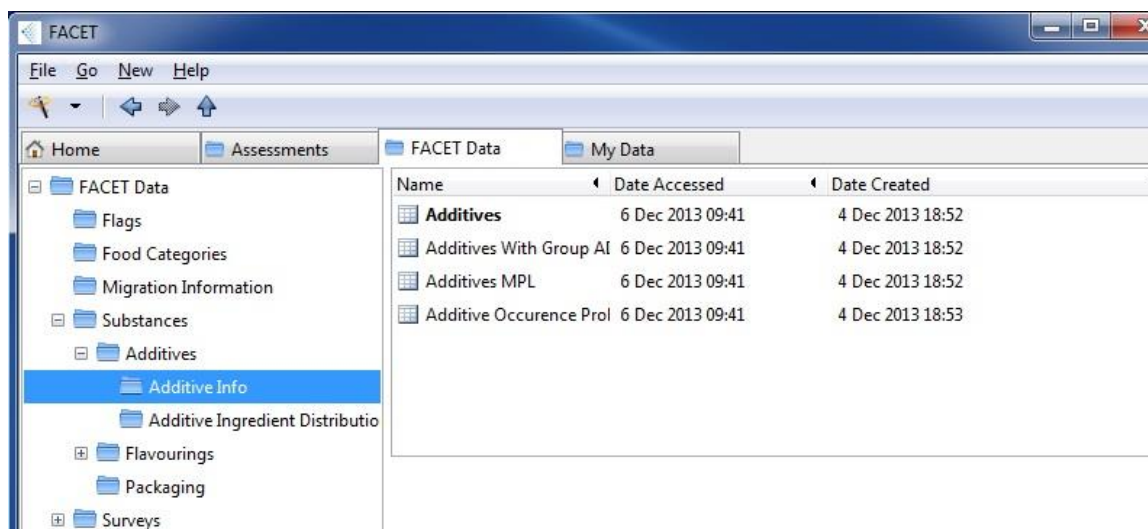


Figure 53: Additive Info Folder.

Additives MPL: A table of Maximum Permitted Levels (MPLs) for the FACET food categories and flag settings, as well as the calculated probability of addition.

The MPL values in this table can be changed, in order to assess the impact of varying the MPL values in an exposure assessment. The field that can be edited is in white. In order to restore the default MPLs, click the “Restore Default” icon in the tool bar.

	Additive Tier 1	FACET Code	FACET Description	Eu Code	Additive Name	Default Maxim...	Maximum Perm...
1	NULL	A.1.1.1.1	Sterilised and UHT milk	E338	Phosphoric acid	1000.0	1000
2	NULL	A.1.1.1.1	Sterilised and UHT milk	E339	Sodium phosphates	1000.0	1000
3	NULL	A.1.1.1.1	Sterilised and UHT milk	E340	Potassium phosphates	1000.0	1000
4	NULL	A.1.1.1.1	Sterilised and UHT milk	E341	Calcium phosphates	1000.0	1000
5	NULL	A.1.1.1.1	Sterilised and UHT milk	E343	Magnesium phosphates	1000.0	1000
6	NULL	A.1.1.1.1	Sterilised and UHT milk	E450	Diphosphates	1000.0	1000
7	NULL	A.1.1.1.1	Sterilised and UHT milk	E451	Triphosphates	1000.0	1000
8	NULL	A.1.1.1.1	Sterilised and UHT milk	E452	Polyphosphates	1000.0	1000
9	NULL	A.1.1.1.3	UHT goat milk	E331	Sodium citrates	4000.0	4000
10	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E425	Konjac gum and glucom	10000.0	10000.0
11	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E620	Glutamic acid	10000.0	10000.0
12	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E621	Monosodium glutamate	10000.0	10000.0
13	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E622	Monopotassium glutama	10000.0	10000
14	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E623	Calcium diglutamate	10000.0	10000
15	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E624	Monoammonium glutam	10000.0	10000
16	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E625	Magnesium diglutamate	10000.0	10000
17	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E626	Guanylic acid	500.0	500
18	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E627	Disodium guanylate	500.0	500
19	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E628	Dipotassium guanylate	500.0	500
20	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E629	Calcium guanylate	500.0	500
21	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E630	Inosinic acid	500.0	500
22	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E631	Disodium inosinate	500.0	500
23	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E632	Dipotassium inosinate	500.0	500
24	NULL	A.1.1.2.2	Sterilised buttermilk (unfl)	E633	Calcium inosinate	500.0	500

Figure 54: Additive MPL Table



Figure 55: Restore Default Icon

Additives Occurrence Probabilities: Database of occurrence probabilities of for FACET food categories.

Additives

The Additives table contains information on all the different additives in FACET. Clicking on the table once will bring up a preview in the bottom right pane, showing a search box for browsing different fields. The table contains the following fields:

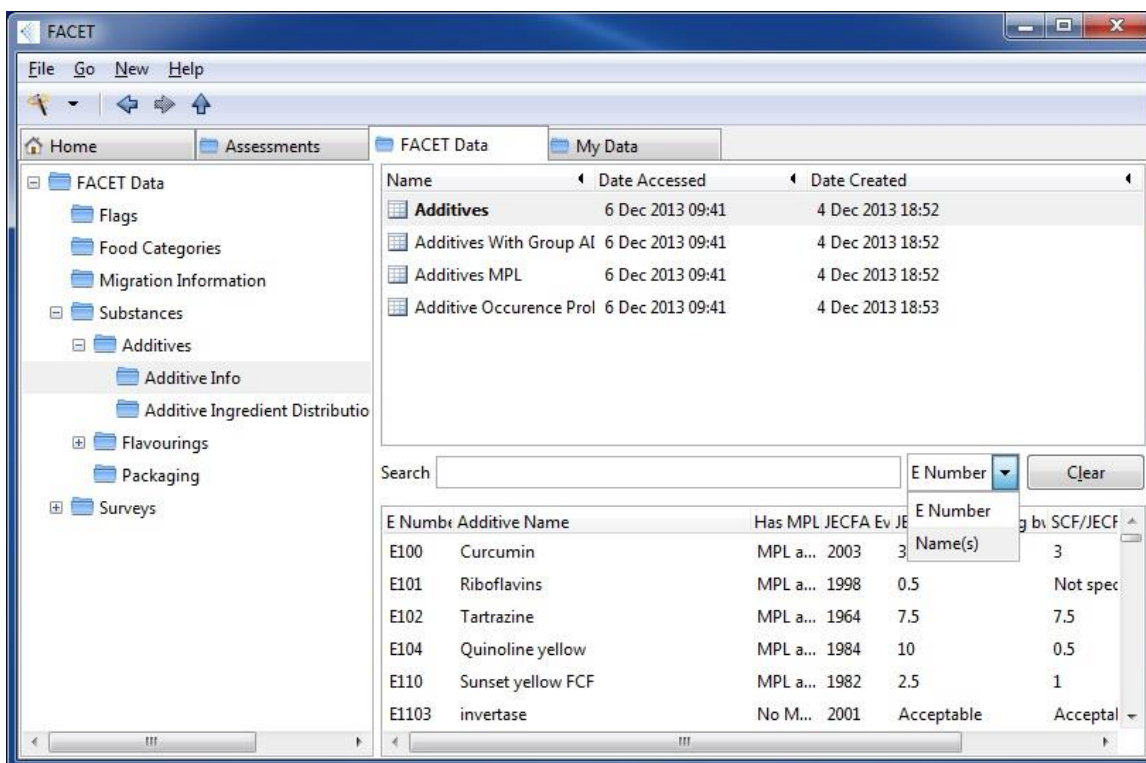


Figure 56: Additive table search box.

- **E Number:** Number given by the EU. This is the unique identifier of the additive.
- **Name:** The name(s) of the additive.
- **JECFA ADI:** Acceptable Daily Intake. This field takes a combination of numbers and letters. Units are listed in mg/kg bw, unless otherwise specified.
- **JECFA Evaluation:** Numerical field, showing the evaluation date. Entries are in a four digit year-type format (e.g. 1991).
- **SCF/EFSA ADI:** Acceptable Daily Intake. This field takes a combination of numbers and letters. Units are listed in mg/kg bw, unless otherwise specified.
- **SCF/EFSA Evaluation:** Numerical field, showing the evaluation date. Entries are in a four digit year-type format (e.g. 1991).

Additive Ingredient Distributions

This folder contains distributions of MPL concentration values for different combinations of food categories and flag settings. The distributions are used to account for the fact that an additive MPL may be set for a component of a food, e.g. in a topping. These distributions are reference in the MPL database.

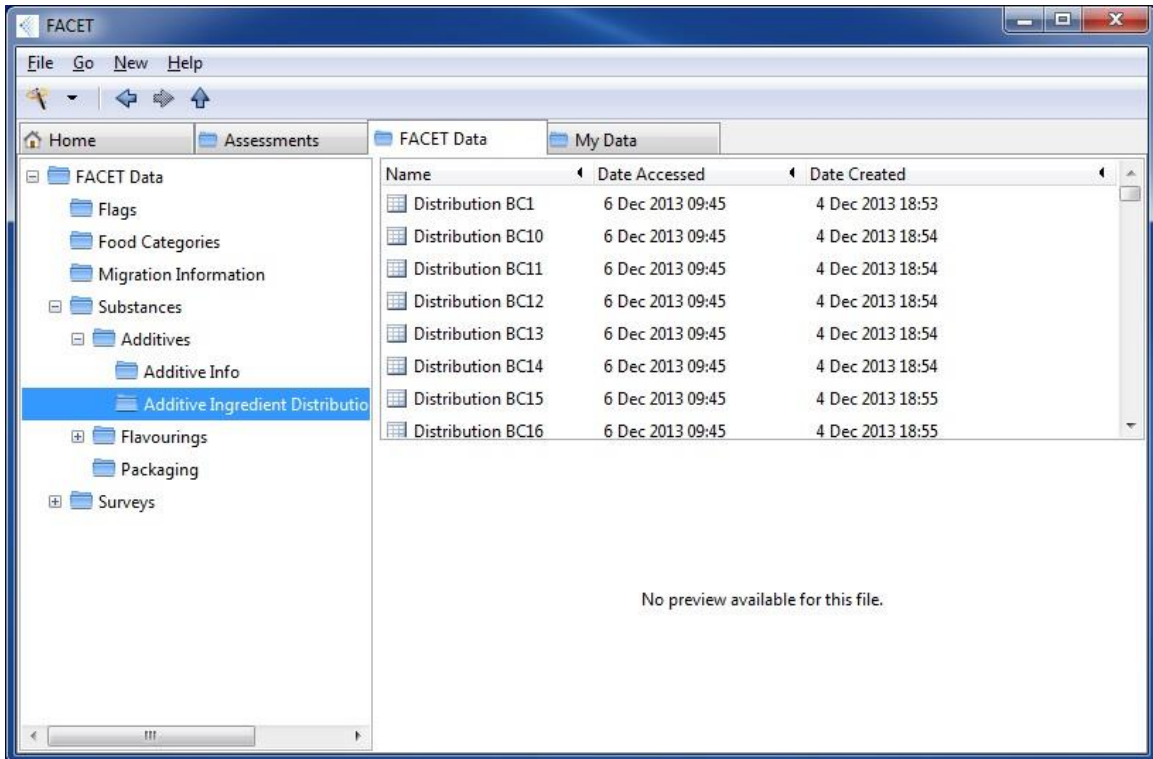


Figure 57: Additive Ingredient Distribution.

Packaging

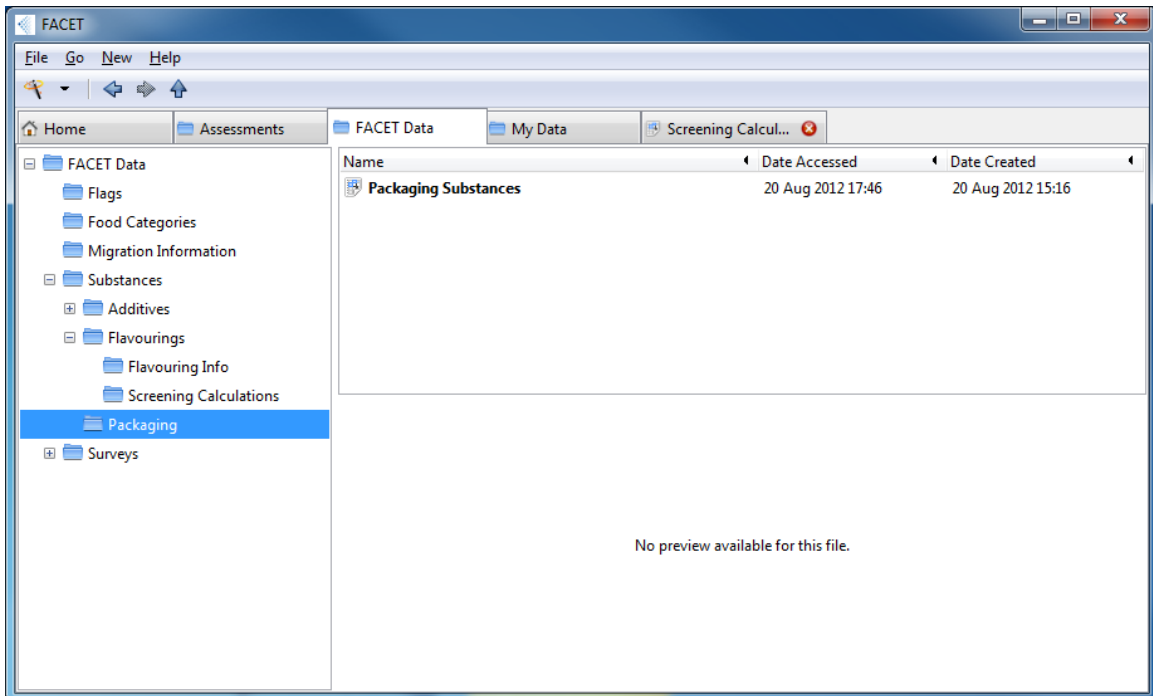


Figure 58: Packaging Folder.

The packaging folder contains one table called Packaging Substances, showing a complete list of all the packaging substances available in FACET. The table contains the following fields:

- **FACET ID:** This is strictly a four digit number with no leading zeros, e.g. “1021”. This is the unique identifier of the migrant.
- **CAS Number:** This is strictly of the form [up to 7 digits]-[2 digits]-[1 digit], e.g. “64-17-5”, or “0000064-17-5”.
- **Chemical Name:** The chemical name(s) of the substance.
- **Alternative Name:** Any other alternative names that might be associated with the substance.
- **Molecular Weight:** Molecular weight of the migrant. Strictly a numeric field.

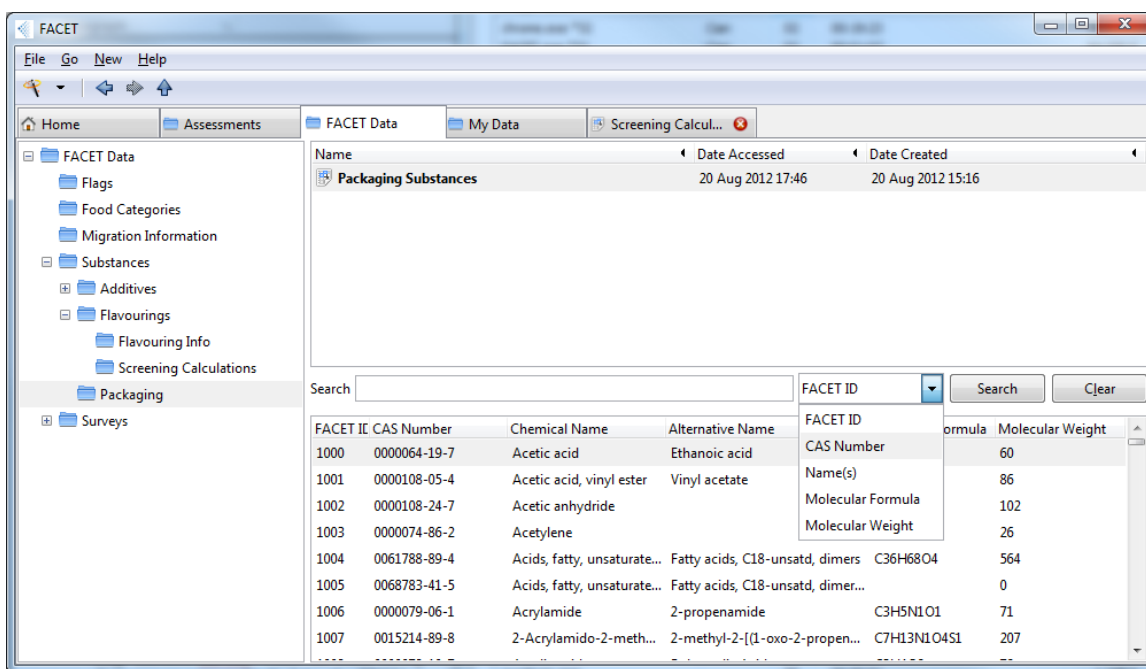


Figure 59: Packaging table search box.

Surveys

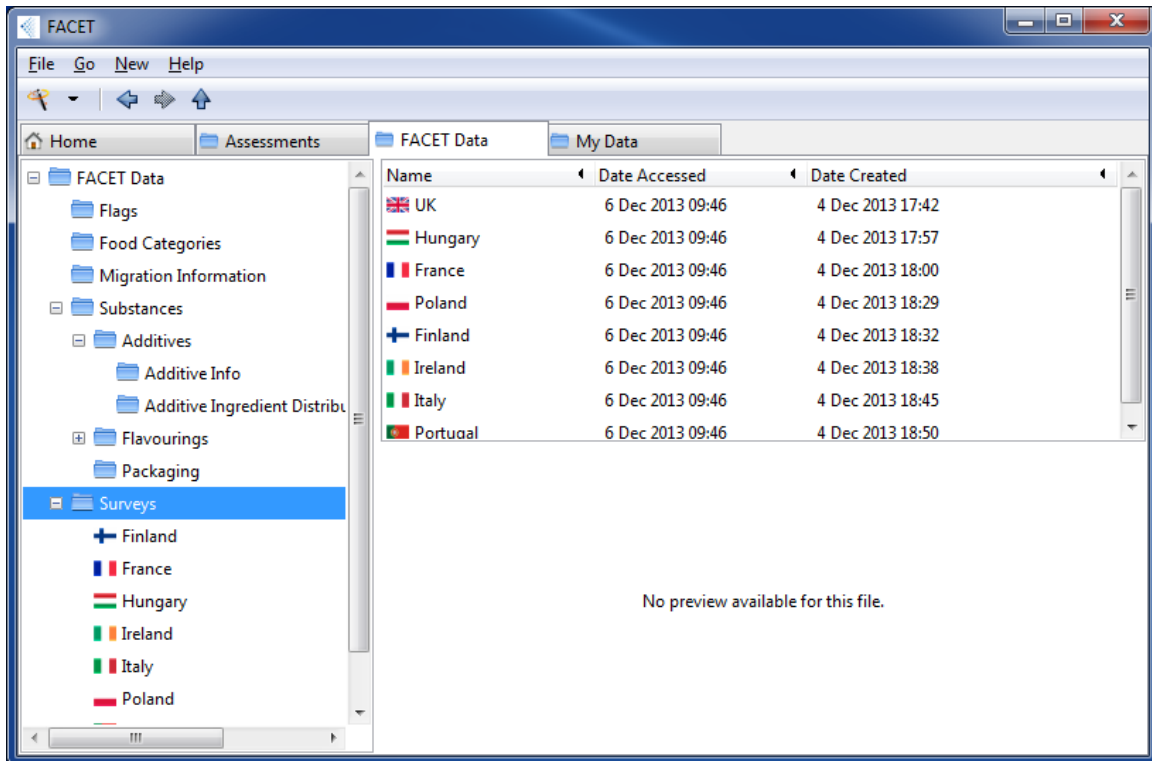


Figure 60: Surveys folder.

This allows you to view the various surveys available in FACET. The available surveys are the same as those that appear in Step 7 of the New Assessment Wizard. The visible fields are:

- **Name:** The name of the survey.
- **Years:** The years in which the survey was carried out.
- **Subjects:** The number of subjects in the survey.
- **Age Range:** The range of ages of subjects in the survey.
- **Methodology:** The methodology used to carry out the survey.
- **Record:** The type of dietary records that appear in the survey.

The screenshot shows the FACET software interface. On the left is a navigation tree with categories like 'Substances' and 'Surveys'. The 'Surveys' category is expanded to show various countries including UK. The main area displays a table of surveys with columns for Name, Row Count, Date Accessed, and Date Created. The 'UK NDNS 2000 19-64' survey is selected. Below the table is a 'Survey Information' panel with the following details:

Survey Information	
Name:	UK NDNS 2000 19-64
Years:	2000/2001
Subjects:	1724
Age Range:	19-64
Methodology:	7 day weighed food diary
Record:	Person/Day/Eating occasion/Food item

Figure 61: Visible fields in survey.

My Data

The My Data tab is where you can create, view and edit your own data that can be used in exposure assessments. You can organise your data in a similar fashion to any file manager (e.g. Windows Explorer).

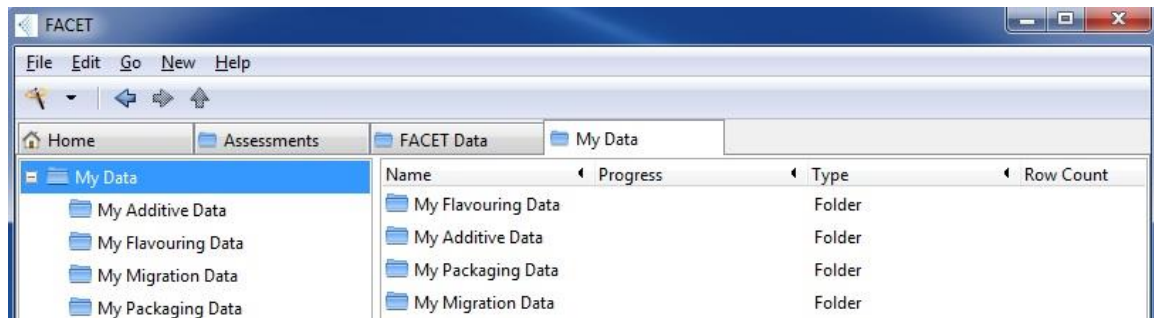


Figure 62: My Data Tab.

Managing Data

Navigating about the data manager

The My Data Tab is implemented in a two pane layout. In the left hand pane is the folder tree, which shows the hierarchy of your folders. The right-hand pane displays the contents of the current folder.

To navigate about the data manager, you can either:

1. Use the “Back”, “Forward”, and “Up” buttons in the tool bar.
2. Click on the folder whose contents you want to view in the folder tree in the left panel.

The folder structure in the left hand panel will expand or collapse to show where in the file manager you are currently viewing.

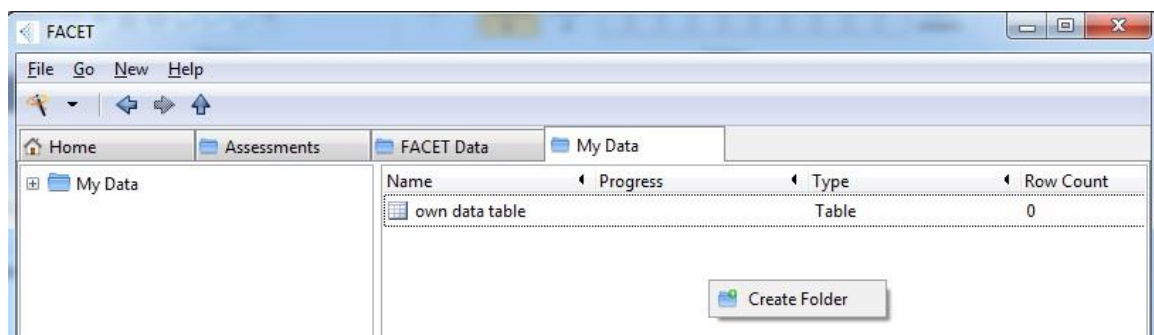


Figure 63: Example of own data table and creating new folder.

Creating a new folder

1. To create a new folder, right click on where you want to create it in the right pane and select “Create Folder”.
2. This will bring up a dialogue box into which you can enter the name of the new folder.
3. After entering the name of the new folder, click on “OK” and the new folder will be created.

Renaming a folder

1. To rename a folder, right click on the folder you want to rename and select “Rename”. Alternatively, you can select the folder and choose “Rename” from the Edit menu.
2. This will bring up a dialogue into which you can enter the new name of the folder. Enter the new name of the folder into the dialogue and click on “Rename”.

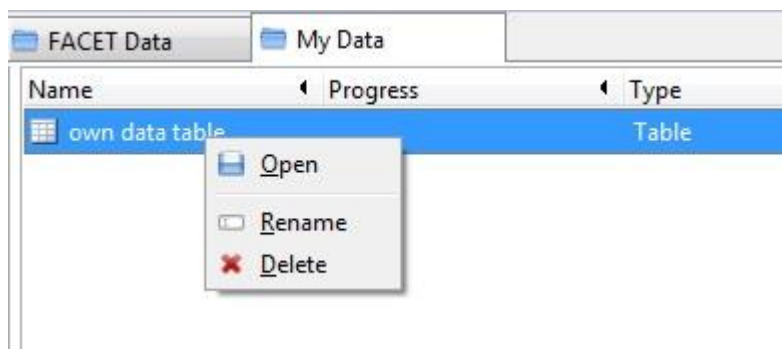


Figure 64: Renaming a folder.

Deleting a folder

1. To delete a folder, right click on the folder you want to rename and select “Delete”. Alternatively, you can select the folder and choose “Delete” from the Edit menu.

New Table Wizard

To create a new table in the My Data tab, you can use the New Table Wizard. This can be selected from the “New” menu or by clicking on the wizard icon and selecting “New Table”. There are three steps to complete:

1. **Substance Type:** Select whether the table is for a new additive, flavouring, or packaging substance.
2. **Select Substance:** Select the substance that will be used for the assessment.
3. **Table Options:** Select the name and location of the table in the My Data tab.

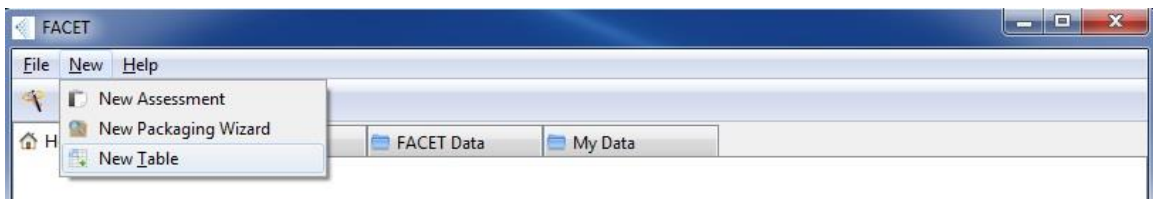


Figure 65: New table wizard using “new” menu.



Figure 66: New table wizard using assessment wizard icon.

The Data Editor

You can edit your own data using the table editor in FACET. To bring up the data editor, double click on a table in the list view. The available operations are listed below.

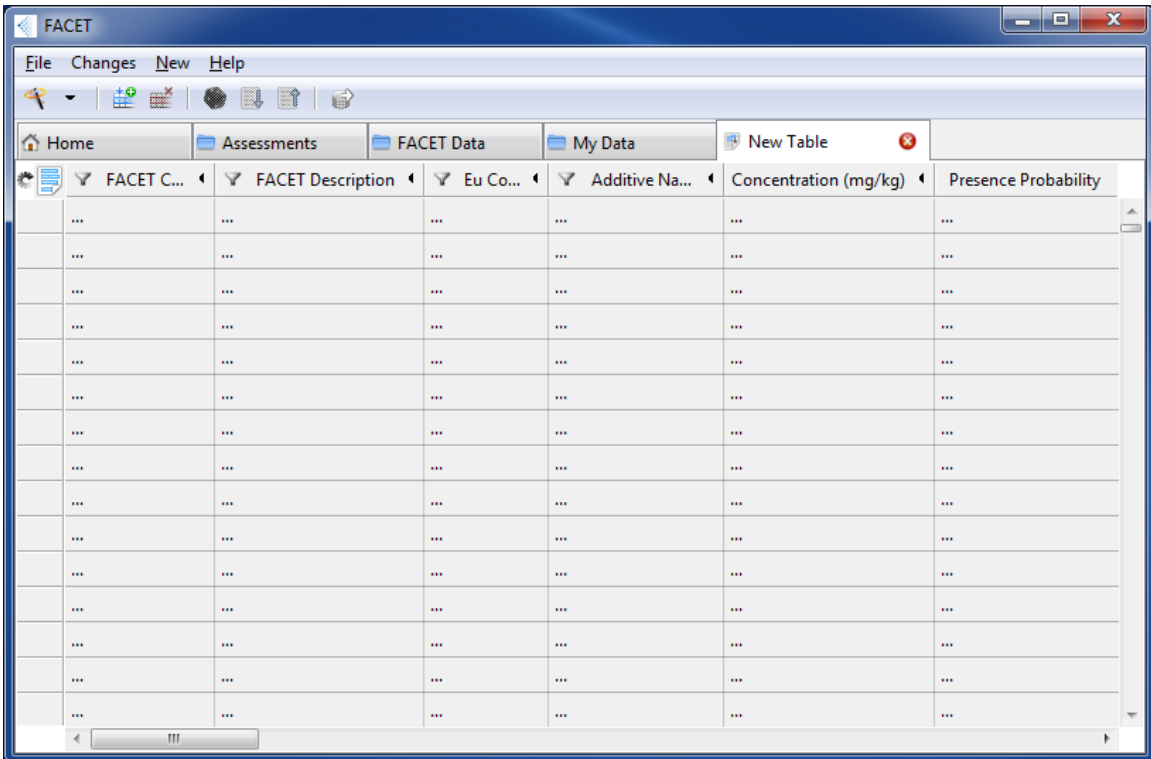


Figure 67: Data Editor.

Insert Row

1. First open the table editor by double-clicking on the table of interest, or selecting the table and selecting "Open" from the file menu.
2. To insert a new row into a table in the table editor, select "Insert row" from the Changes menu, or click on the "Insert row" icon.

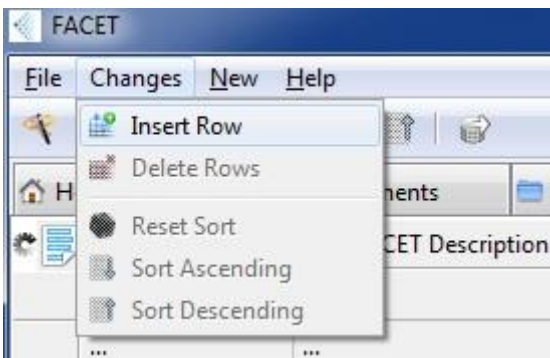


Figure 68: Insert row using changes menu.

3. Changes to the table are saved automatically.

The screenshot shows the FACET software window with a table editor. The table has the following columns: FACET C..., FACET Description, Eu Co..., Additive Na..., Concentration (mg/kg), and Presence Probability. The first row contains the following data: 1, A.1, DAIRY PRODUCTS AND AN, E110, Sunset yellow FCF, NULL, NULL. The rest of the rows are empty, indicated by three dots in each cell.

	FACET C...	FACET Description	Eu Co...	Additive Na...	Concentration (mg/kg)	Presence Probability
1	A.1	DAIRY PRODUCTS AND AN	E110	Sunset yellow FCF	NULL	NULL

Figure 69: Inserting a new row

Delete Row

- 1. First open the table editor by double-clicking on the table of interest, or selecting the table and clicking on the "Open" button from the file menu or pressing Ctrl + O.
- 2. To delete single or multiple rows, first highlight the required rows by clicking on the left hand margin of the relevant rows.

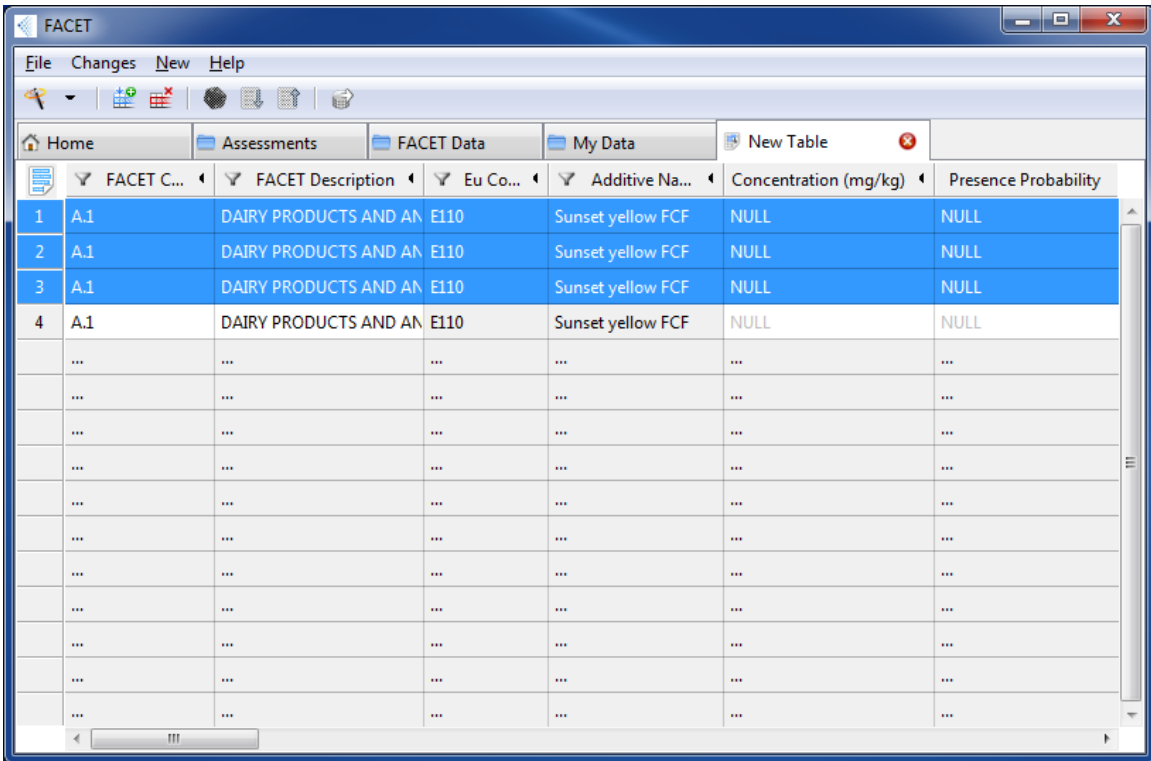


Figure 70: Selecting and deleting multiple rows.

- Multiple rows can be selected by clicking and pressing the Ctrl key.
- To delete the selected rows, click on the "Delete Row" icon, or select "Delete Rows" from the Changes menu.

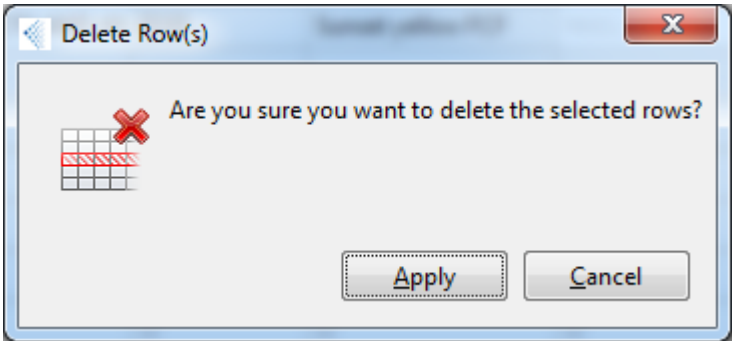


Figure 71: Delete rows.

- Changes to the table are saved automatically.

Entering data

User-defined concentration data requires the four types of information; concentrations, food codes, flag settings, and presence probabilities.

Concentrations

To enter a concentration value for a given row (note that the units are in mg/kg):

1. Double-click on the cell with the header “Concentration”.
2. Entered the concentration data and press return. The value entered can be a number or a parametric distribution.
3. Changes to the table are saved automatically.

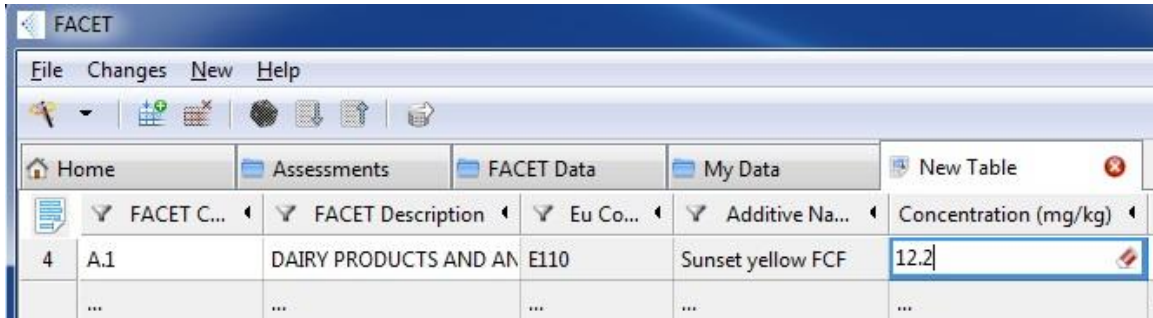


Figure 72: Enter concentration data.

Presence Probabilities

To enter a presence probability for a given row (note that the value should be between 0 and 1):

1. Double-click on the cell with the header “Presence Probability”.
2. Changes to the table are saved automatically.

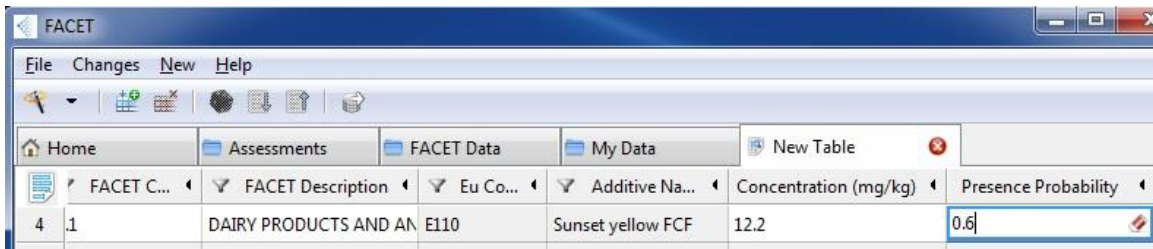


Figure 73: Enter presence probability.

Food Codes

FACET food codes can be entered at any level in the hierarchy, and can be entered by the FACET food code or the FACET food description. To select a FACET food code:

1. Double-click on the cell with either the header “FACET Code” or “FACET Description”, or click on the cell and press return.
2. Select the food category you want. Entries with an arrow show the categories at the lower tier.
3. Depending on which is selected, the “FACET Code” and “FACET Description” will update automatically.
4. Changes to the table are saved automatically.

	FACET C...	FACET Description	Eu Co...
4	A.1	A.1	DUCTS AND AN E110
	A.2	A.1.1	...
	A.3	A.1.2	...
	A.4	A.1.3	...
	A.5	A.1.4	...
	A.6	A.1.5	...
	A.7	A.1.6	...
	A.8
	A.9
	A.10
	A.11
	A.12
	A.13
	A.14

Figure 74: Facet food code hierarchy.

Flag Settings

FACET flag settings can be entered by their number or description. To enter a flag setting at a given setting:

1. Double-click on the cell for the flag you want to set, using the flag description or number, or click on the cell and press return.
2. The list of available options for that cell will appear. Select the one you want.
3. Double-click on the cell you want to enter data into
4. Changes to the table are saved automatically.

Flag 1	Flag 1 Code
Unknown	
Retail incl. over the counter	
Take away / vending / fast food	
Restaurant / canteen	
Homegrown / Homemade	
...	...

Figure 75: Facet flag settings.

Advanced Packaging Interface

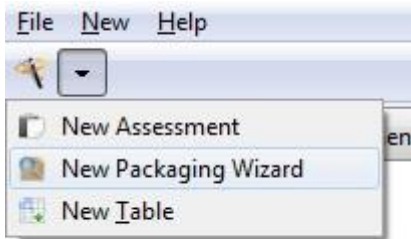


Figure 76: Advanced packaging interface using wizard icon

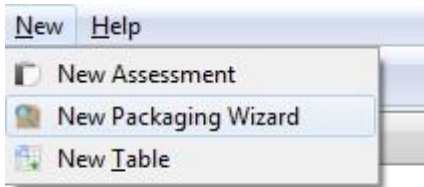


Figure 77: Advanced packaging interface using “new” menu.

The advanced packaging interface can be used to investigate the impact of bringing a new packaging structure, material, or packaging type to the market, from the point of view of consumer exposure. To open the advanced packaging interface, click on the wizard icon and select “New Packaging Assessment”, or select “New Packaging Assessment” from the New menu. There are two assessment types in the New Packaging Wizard:

1. New Pack Type
2. New Metal Pack Type

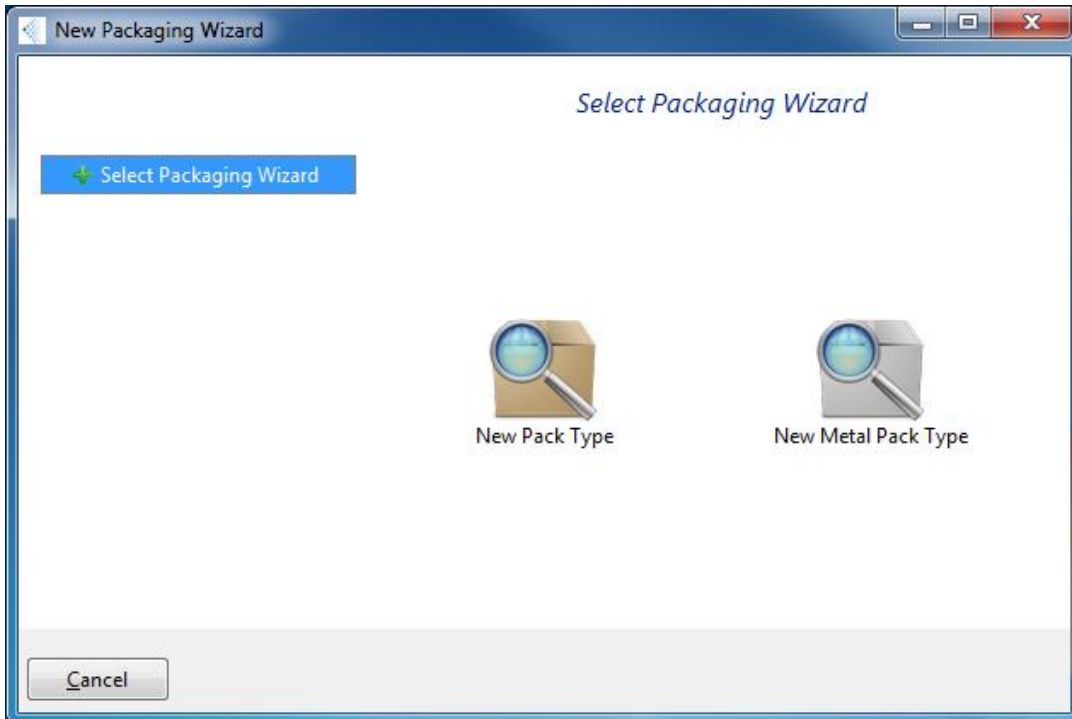


Figure 78: Packaging Assessment home page.

New Pack Type

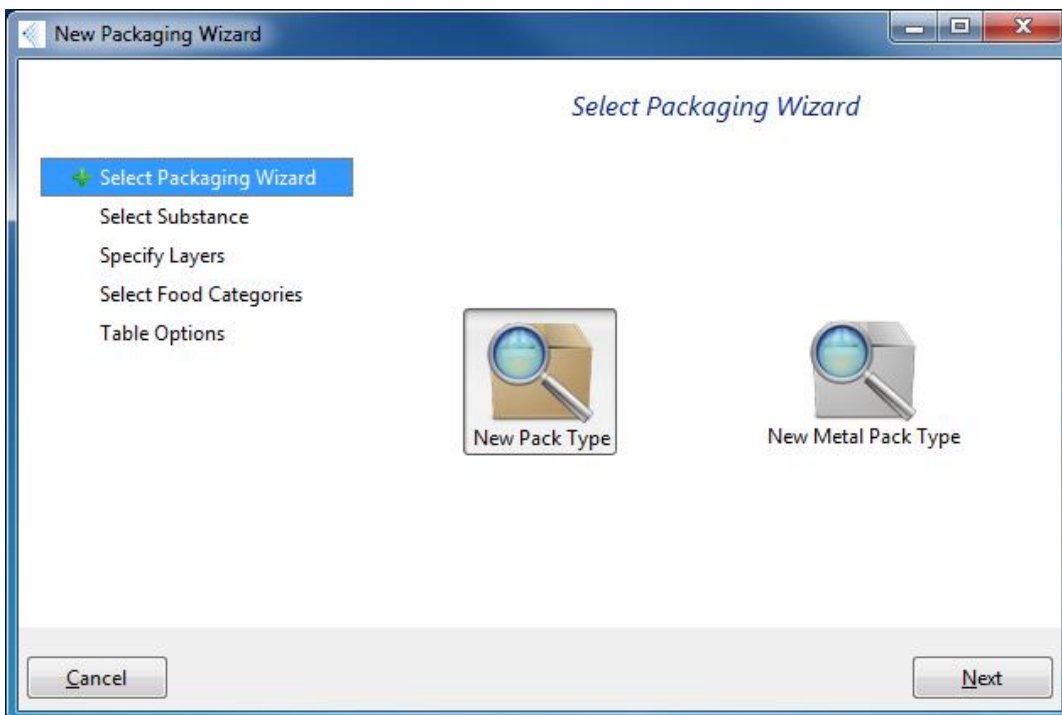


Figure 79: New pack type assessment.

The new structure option assesses the impact of bringing an entire new packaging configuration to market. The predicted migration of an additive from the components in the packaging into relevant foods is assessed and outputted to a database for use in an exposure assessment. There are three steps to complete.

1. Select Substance

Here you can choose the substance whose level of migration you want to assess. You can perform the assessment with a new substance or an existing substance

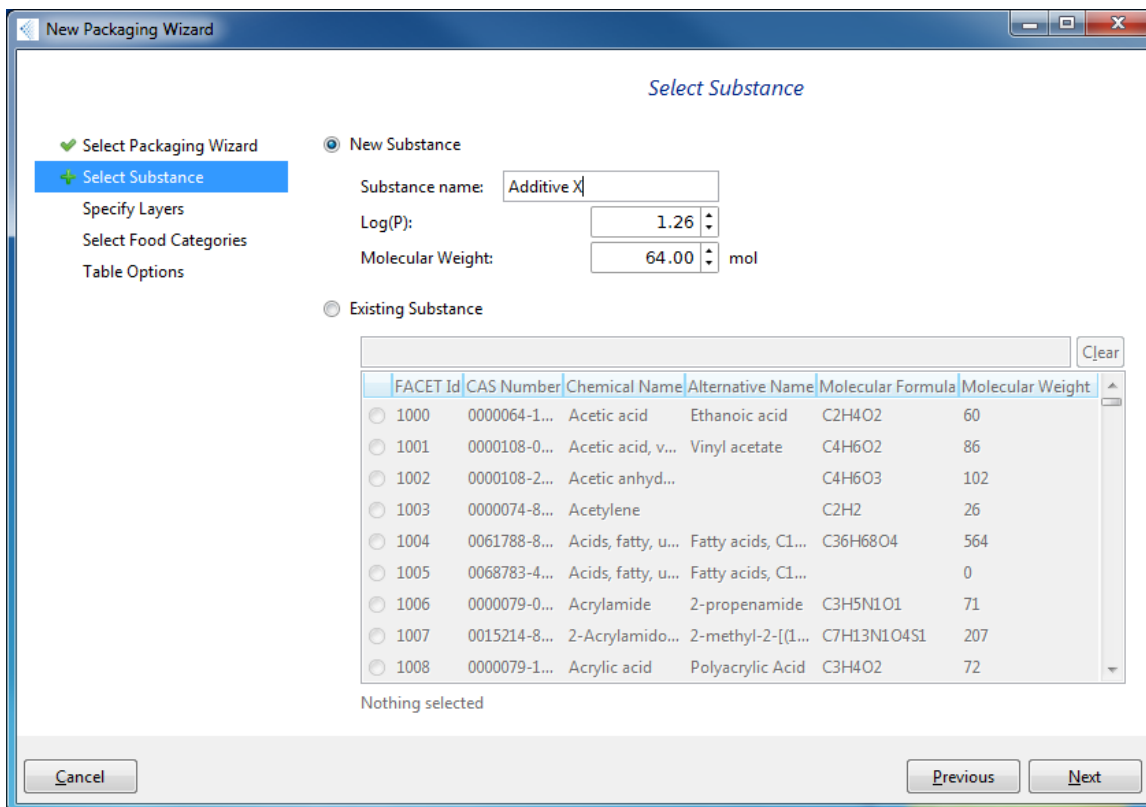


Figure 80: Create new substance

New Substance

1. Enter the name of the additive in the box provided.
2. Enter the Log P of the substance.
3. Enter the molecular weight of the substance.

Existing Substance

1. Search for the name of the substance in the search box provided.
2. Select the substance from the list.

Existing Substance

	FACET Code	CAS Number	Chemical Name	Alternative Name	Molecular Formula	Molecular Weight
<input type="radio"/>	1004	0061788-...	Acids, fatty...	Fatty acids, C...	C36H68O4	564
<input type="radio"/>	1005	0068783-...	Acids, fatty...	Fatty acids, C...		0
<input type="radio"/>	1006	0000079-...	Acrylamide	2-propenamide	C3H5N1O1	71
<input type="radio"/>	1007	0015214-...	2-Acrylamid...	2-methyl-2-[(1...	C7H13N1O4S1	207
<input type="radio"/>	1008	0000079-...	Acrylic acid	Polyacrylic Acid	C3H4O2	72
<input type="radio"/>	1009	0002495-...	Acrylic acid,...	Benzyl acrylate	C10H10O2	162
<input type="radio"/>	1010	0000141-...	Acrylic acid,...	n-Butyl acrylat...	C7H12O2	128
<input type="radio"/>	1011	0002998-...	Acrylic acid,...	sec-Butyl met...	C7H12O2	128
<input type="radio"/>	1012	0001663-...	Acrylic acid,...	tert-Butyl acry...	C7H12O2	128

Nothing selected

Previous

Next

Figure 81: Search for existing substance and submit.

Once all the steps have been completed, click the Submit button.

2. Specify Layers

This is where you specify the type and construction of each component of the packaging being used.

The layers of materials used for the construction of the component can be selected from the list on the left hand side, which also has a search box at the top. The order of the layers is built up from the food layer outwards. To build up the structure:

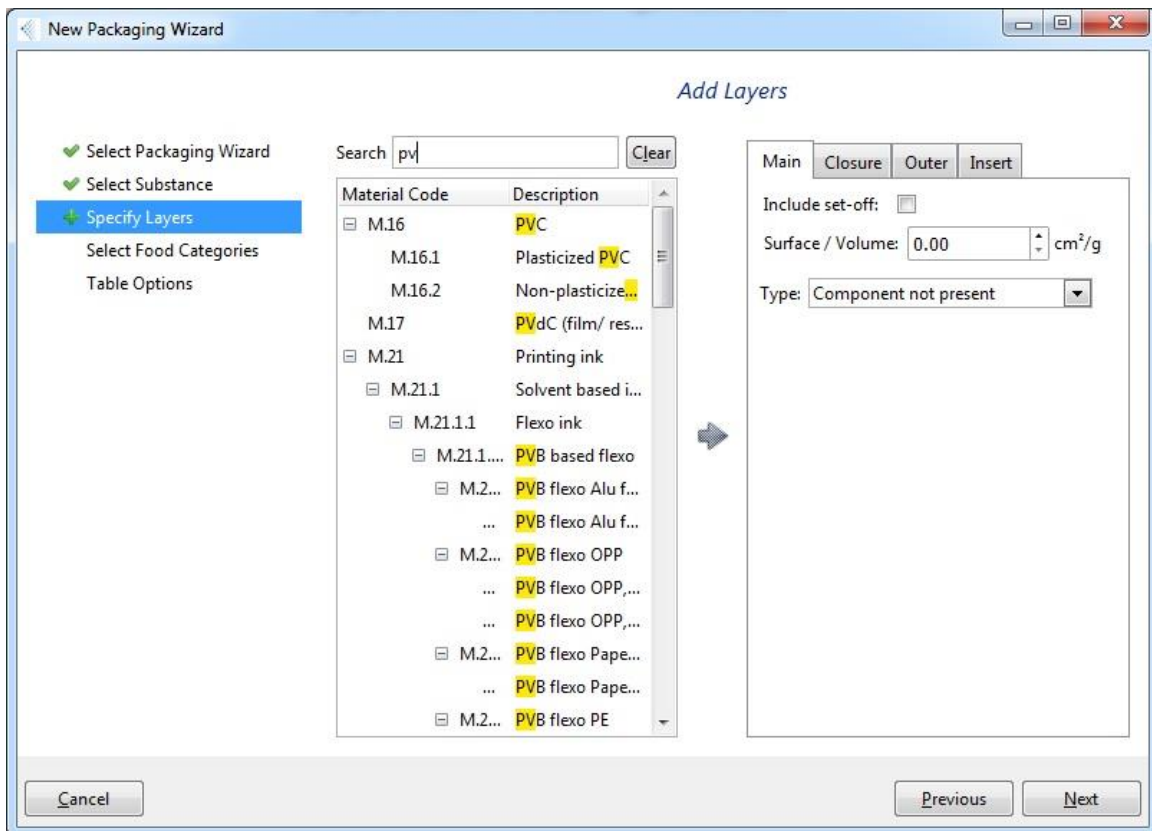


Figure 82: Specify layers search by name.

1. At the top on the right-hand side, there are four tabs. Use these to select whether the packaging has a main, closure, outer, or insert component.
2. The user has the option to select set-off in the assessment. This is achieved by checking the "Include set-off" option.
3. The surface to volume ratio can be specified by entering the appropriate value (in cm²/g) in the box to the right of "Surface/Volume".
4. For each tab, select the component type from the "Type" drop-down menu. If the structure doesn't have a particular component, select "Component not present" from the drop-down menu (selected by default).

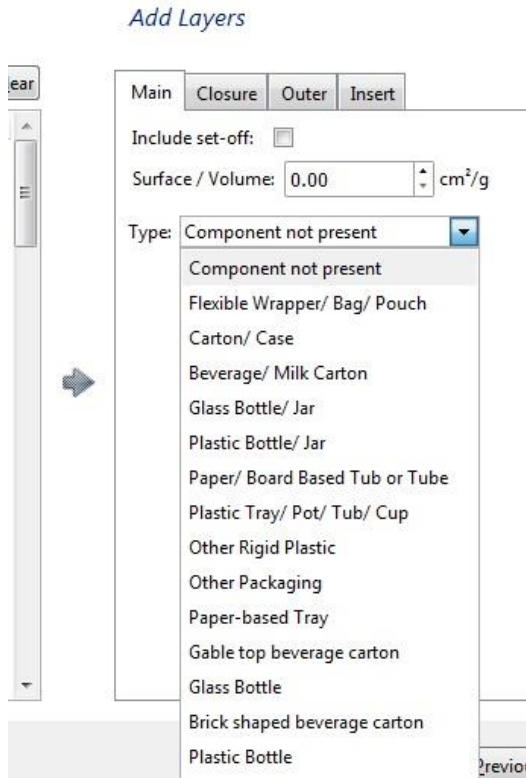


Figure 83: Select component type.

5. Add a material to the structure by selecting it from the list on the left and clicking on the blue arrow to add it to the structure.

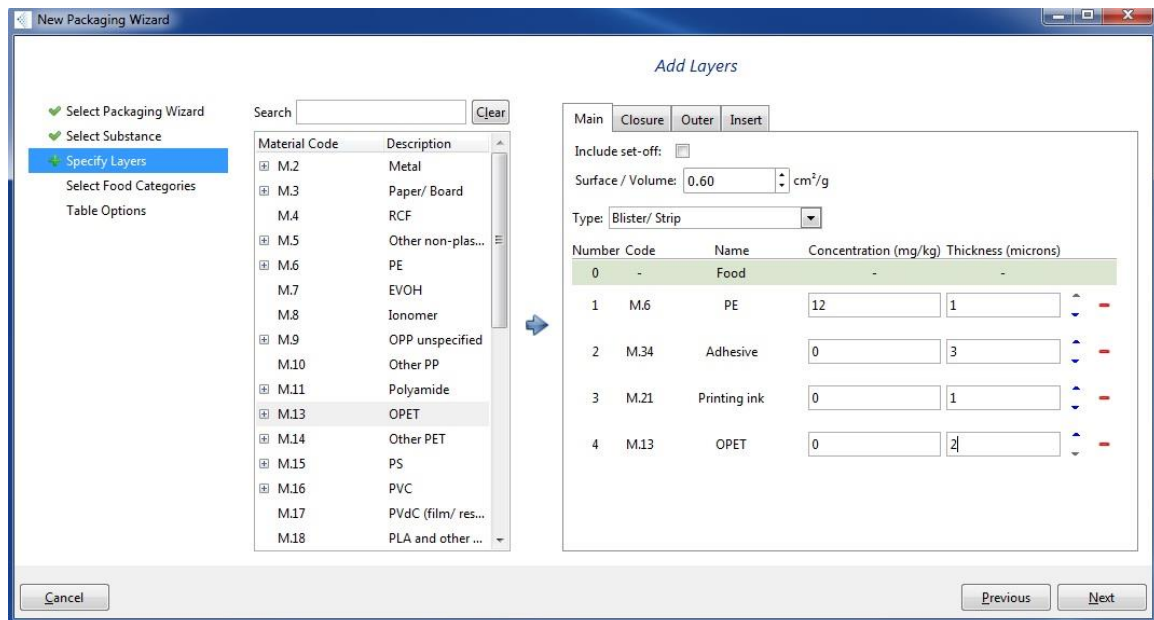


Figure 84: Add a material and specify concentration of additive/thickness of each layer.

6. Specify the concentration of the additive in each layer (in mg/kg) and the thickness of each layer (in microns). This value can also be a parametric distribution.
7. Repeat for all required materials and components.
8. The order of the layers can be re-arranged by using the black up and down arrows next to each material.
9. Materials can also be removed by clicking on the red minus symbol next to each layer.

Main
Closure
Outer
Insert

Include set-off:

Surface / Volume: cm²/g

Type: Blister/ Strip

Number	Code	Name	Concentration (mg/kg)	Thickness (microns)	
0	-	Food	-	-	
1	M.6	PE	<input style="width: 80px;" type="text" value="12"/>	<input style="width: 80px;" type="text" value="1"/>	▲ ▼
2	M.34	Adhesive	<input style="width: 80px;" type="text" value="0"/>	<input style="width: 80px;" type="text" value="3"/>	▲ ▼
3	M.21	Printing ink	<input style="width: 80px;" type="text" value="0"/>	<input style="width: 80px;" type="text" value="1"/>	▲ ▼
4	M.13	OPET	<input style="width: 80px;" type="text" value="0"/>	<input style="width: 80px;" type="text" value="2"/>	▲ ▼

Figure 85: Use arrows to re-arrange layers and red minus to remove.

3. Select Food Categories

This is where you select the foods used for the assessment and the times and temperatures the packaging is in contact with the food. Up to five time and temperature regimes can be selected.

1. The foods used for the assessment can be selected from the list, which has a search box at the top. Once a food is selected, click on the “Create” button. This will open a new panel on the left-hand side.

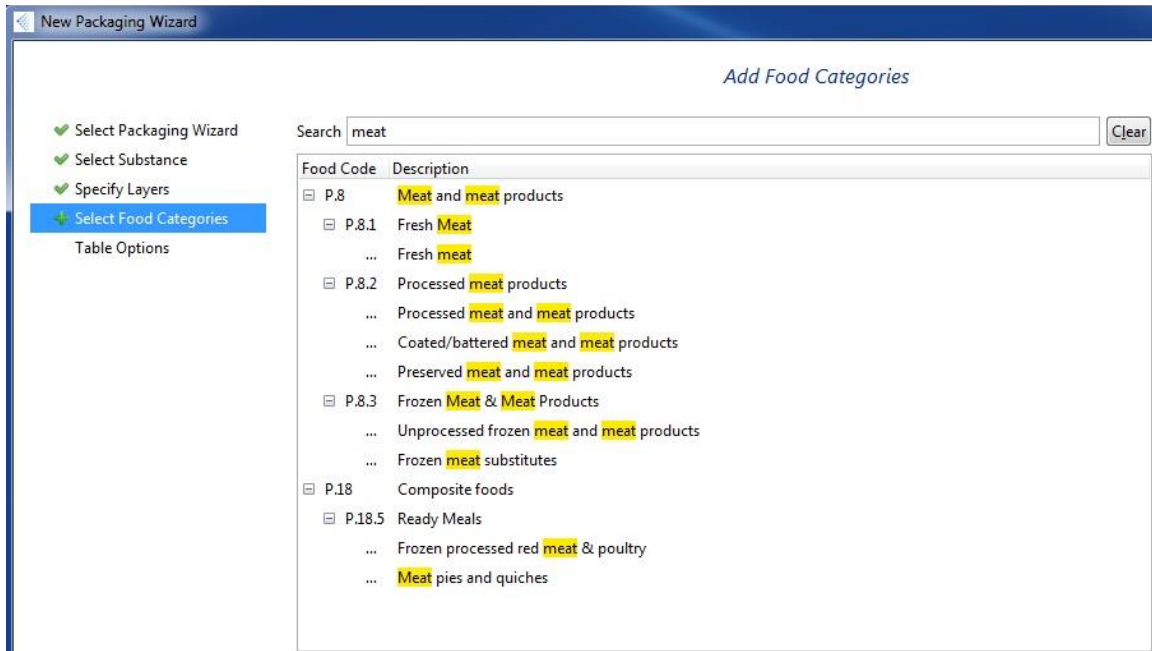


Figure 86: Search for food category.

2. At the top of the new panel, select the market share the component has in that food category by entering the appropriate value in the box.
3. Enter the volume of the pack the new component will be used with.
4. Enter the Pack size in grams.
5. In the bottom box enter the upper and lower limits of the times and temperatures the food/component combination will undergo. The units can be specified in the drop-down menus on the right-hand side.
6. Additional time-temperature regimes can be added by clicking on the green plus symbol on the right-hand side.
7. Time-temperature regimes can be removed by clicking on the red minus symbol on the right-hand side.

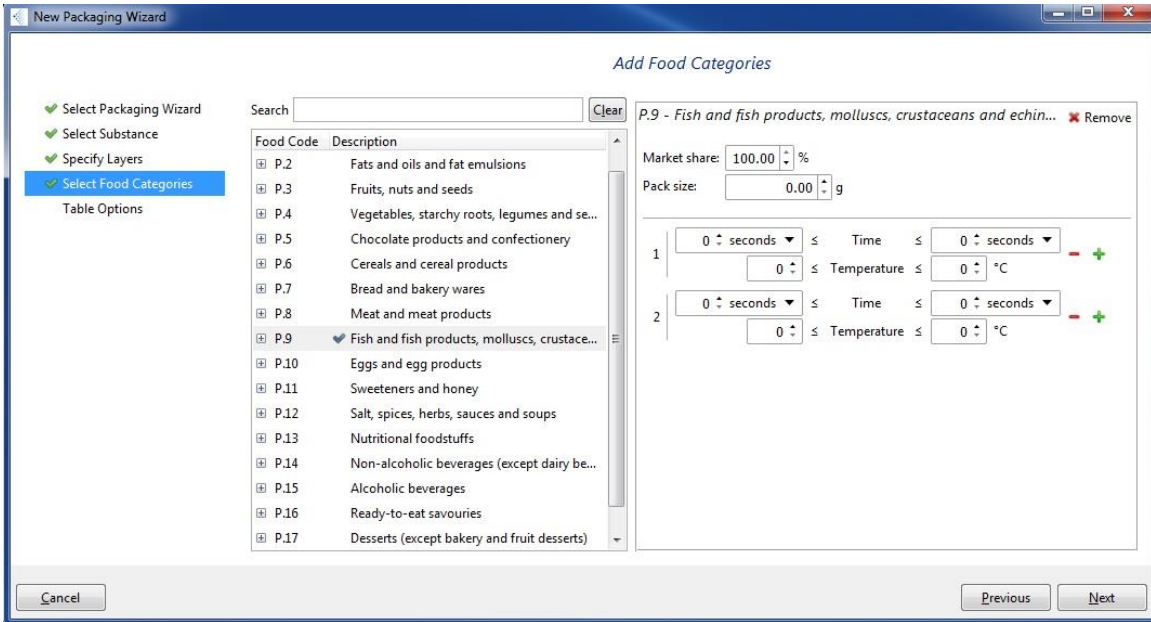


Figure 87: Create food category.

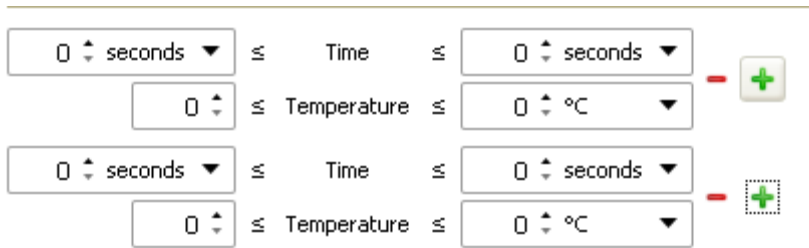


Figure 88: Additional time and temperature added using plus symbol. Remove using minus.

If desired, factory storage can also be modelled. To do this, simply click the “Include factory storage” checkbox.

4. Table Options

This step presents you with a summary of the current choices of substances, populations and food categories for the assessment.

After reviewing the choices, you can choose to start an assessment using the “Submit” button at the bottom right of the window.

Equally, you may wish to make changes to the selections. Navigation to the appropriate steps to do this is easily achieved with the buttons on the left of the tab.

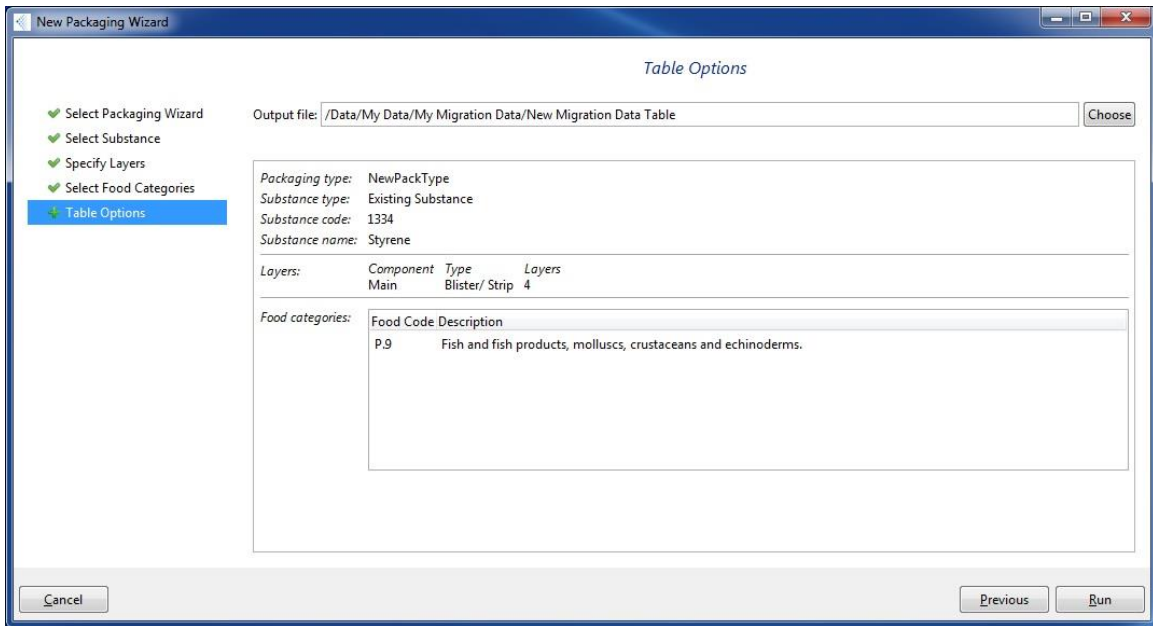


Figure 89: Table Options

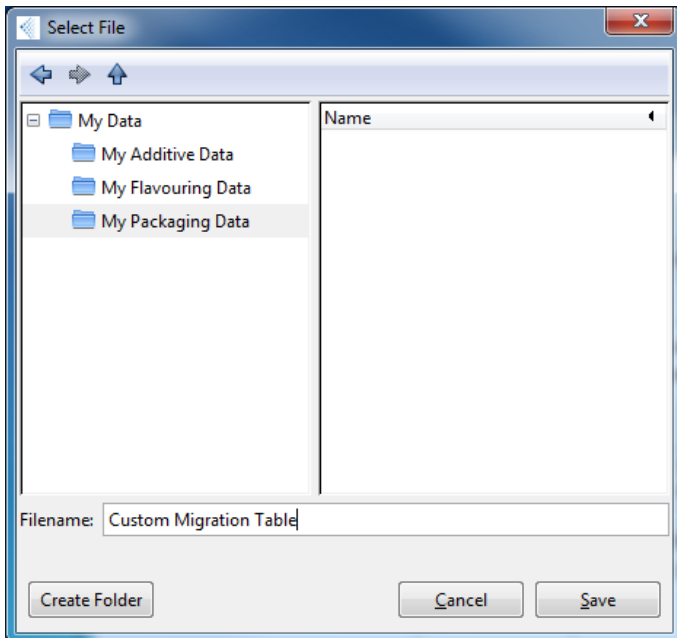


Figure 90: Saving custom migration to a file.

Metal Pack Type

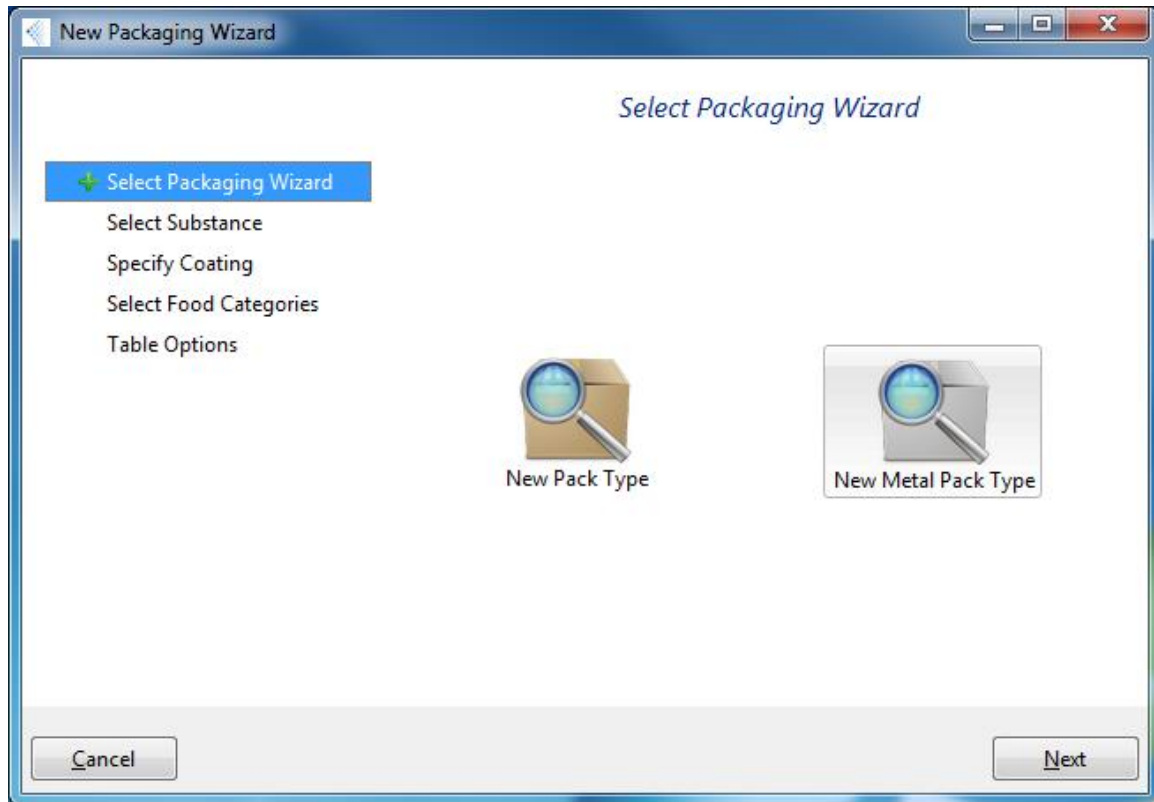


Figure 91: New metal pack type assessment.

The new metal structure feature assesses the impact of bringing an entire new metal packaging configuration to market. The predicted migration of an additive from the components in the metal packaging into relevant foods is assessed and outputted to a database for use in an exposure assessment. There are three steps to complete.

1. Select Substance

Here you can choose the substance whose level of migration you want to assess. You can perform the assessment with a new substance or an existing substance. In both cases, you need to enter the substance concentration in the material at the bottom of the page, in mg/kg. This value can be a concentration or a parametric distribution.

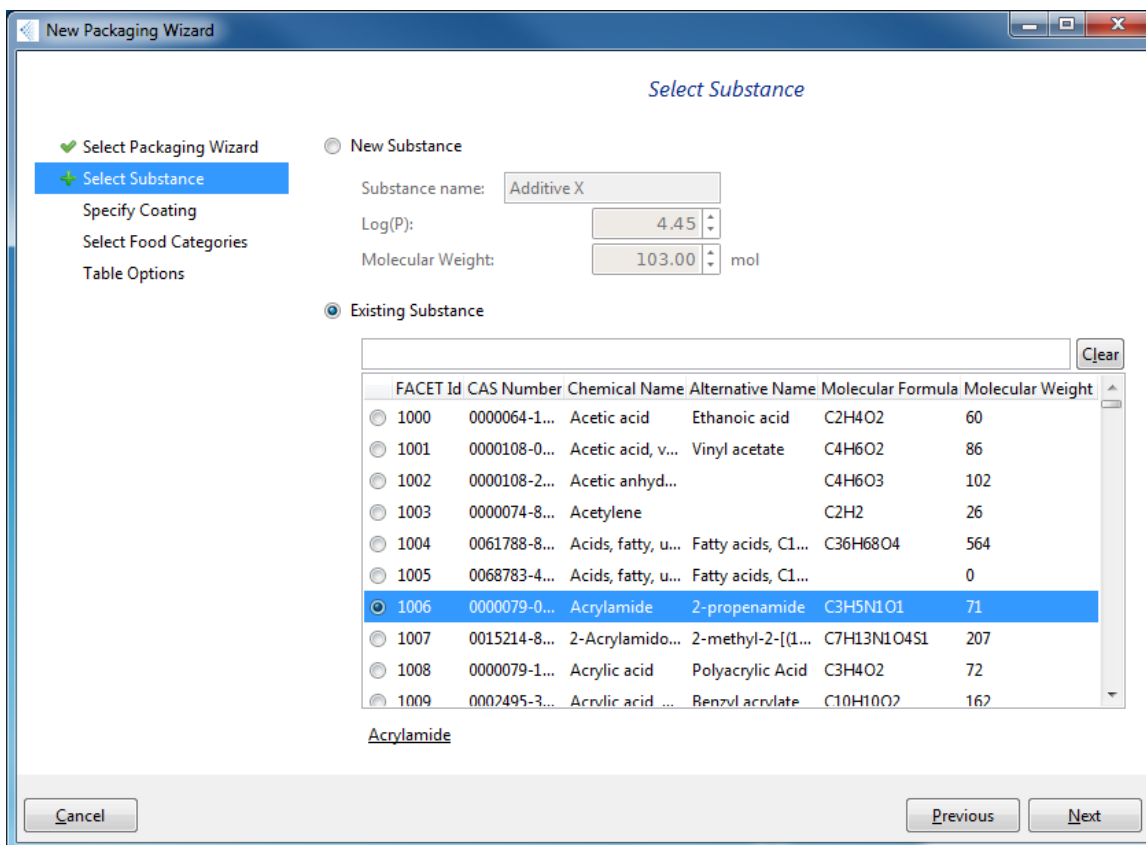


Figure 92: Create new substance.

New Substance

1. Enter the name of the additive in the box provided.
2. Select whether the substance is polar, medium polar, or non-polar from the drop-down menu.
3. Enter the molecular weight of the substance.

Existing Substance

1. Search for the name of the substance in the search box provided.
2. Select the substance from the list.

Existing Substance

	FACET Code	CAS Number	Chemical Name	Alternative Name	Molecular Formula	Molecular Weight
<input type="radio"/>	1004	0061788-...	Acids, fatty...	Fatty acids, C...	C ₃₆ H ₆₈ O ₄	564
<input type="radio"/>	1005	0068783-...	Acids, fatty...	Fatty acids, C...		0
<input type="radio"/>	1006	0000079-...	Acrylamide	2-propenamide	C ₃ H ₅ N ₁ O ₁	71
<input type="radio"/>	1007	0015214-...	2-Acrylamid...	2-methyl-2-[(1...	C ₇ H ₁₃ N ₁ O ₄ S ₁	207
<input type="radio"/>	1008	0000079-...	Acrylic acid	Polyacrylic Acid	C ₃ H ₄ O ₂	72
<input type="radio"/>	1009	0002495-...	Acrylic acid,...	Benzyl acrylate	C ₁₀ H ₁₀ O ₂	162
<input type="radio"/>	1010	0000141-...	Acrylic acid,...	n-Butyl acrylat...	C ₇ H ₁₂ O ₂	128
<input type="radio"/>	1011	0002998-...	Acrylic acid,...	sec-Butyl met...	C ₇ H ₁₂ O ₂	128
<input type="radio"/>	1012	0001663-...	Acrylic acid,...	tert-Butyl acry...	C ₇ H ₁₂ O ₂	128

Nothing selected

Previous

Next

Figure 93: Search for existing substance.

Once all the steps have been completed, click the Run button.

2. Specify Coatings

This is where you specify the type and construction of each component of the packaging being used. The layer of material used for the coating of the component can be selected from the list on the left hand side, which also has a search box at the top. Only the food contact layer is required. To build up the structure:

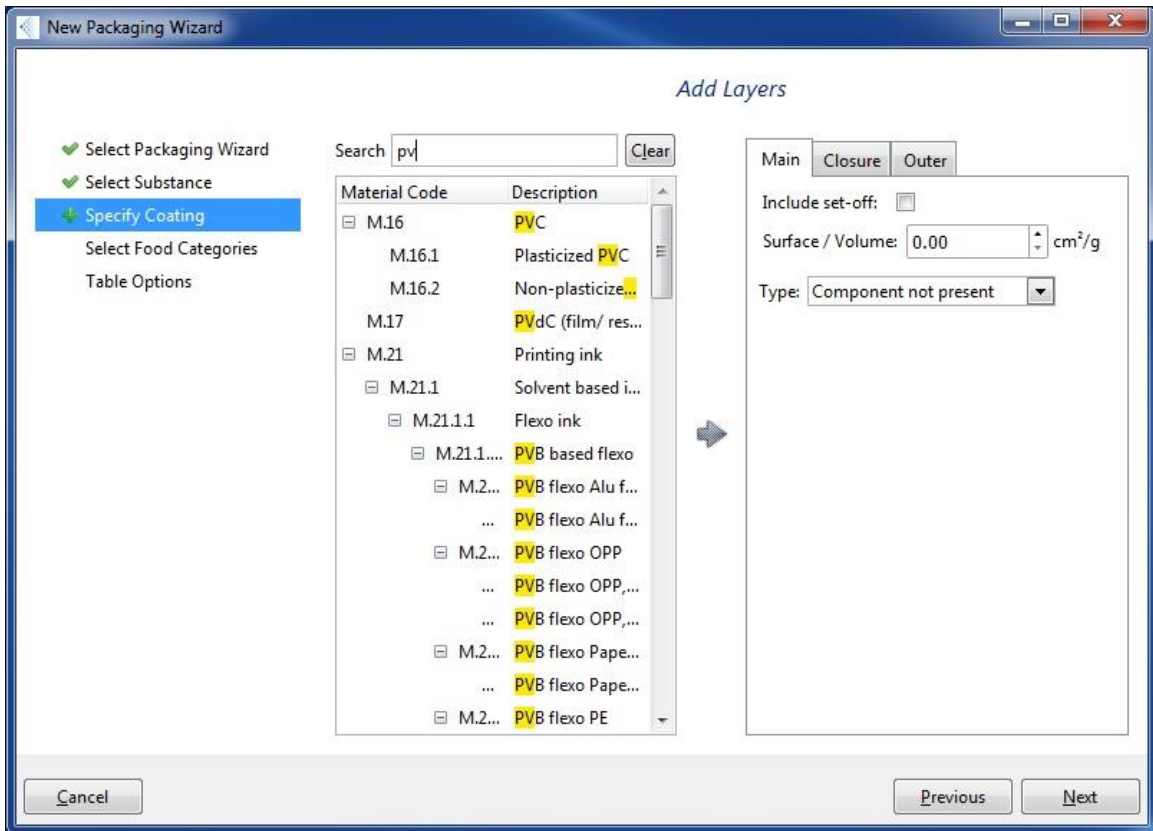


Figure 94: Specify layers- search by name.

1. At the top, there are three tabs. Use these to select whether the component is a main, closure, or outer component.
2. Select the component type from the “Type” drop-down menu.

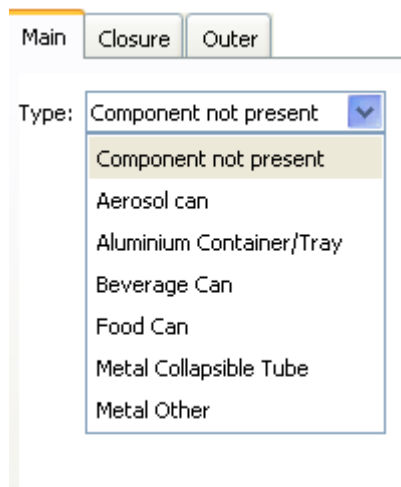


Figure 95: Select component type.

3. Add a material to the structure by selecting it from the list and clicking on the blue arrow to add the structure.

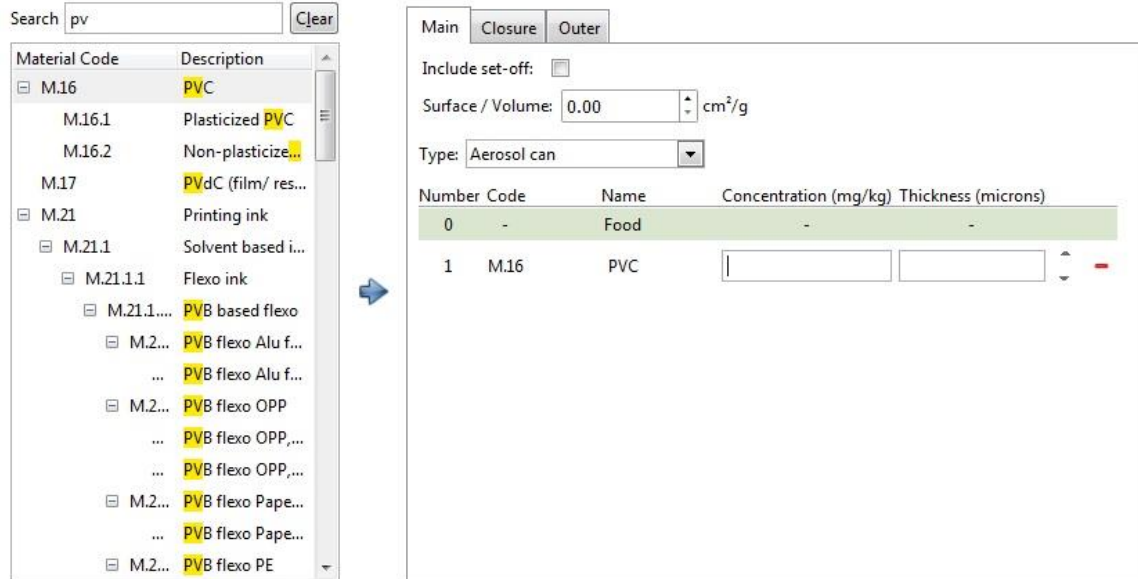


Figure 96: Add a material and specify concentration of additive/thickness of each layer.

4. Specify the concentration of the additive in each layer (in mg/kg) and the thickness of each layer (in microns).

3. Select Food Categories

This is where you select the foods used for the assessment and the rate of extraction of the additive from the can coating.

1. The foods used for the assessment can be selected from the list, which has a search box at the top. Once a food is selected, click on the “Create” button. This will open a new panel on the left-hand side.

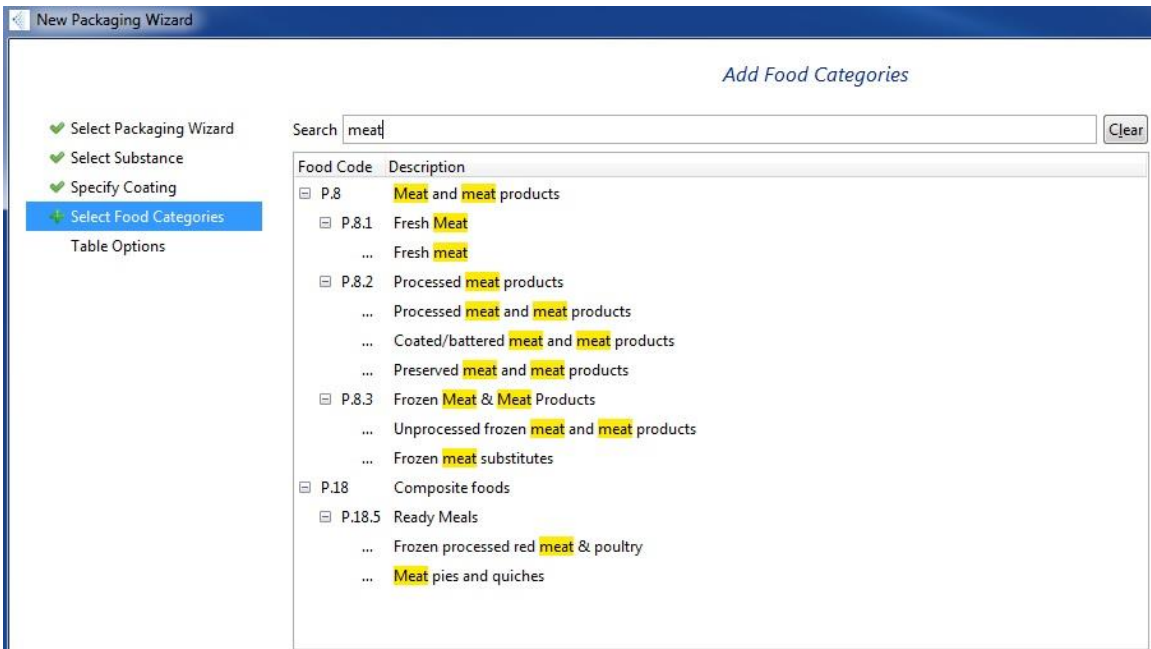


Figure 97: Search for food category.

2. At the top of the new panel, select the market share the component has in that food category by entering the appropriate value in the box.
3. Enter the volume of the pack the new component will be used with.
4. Enter the rate of migration of the substance into the food (in mg/cm^2). This value can also be a parametric distribution.

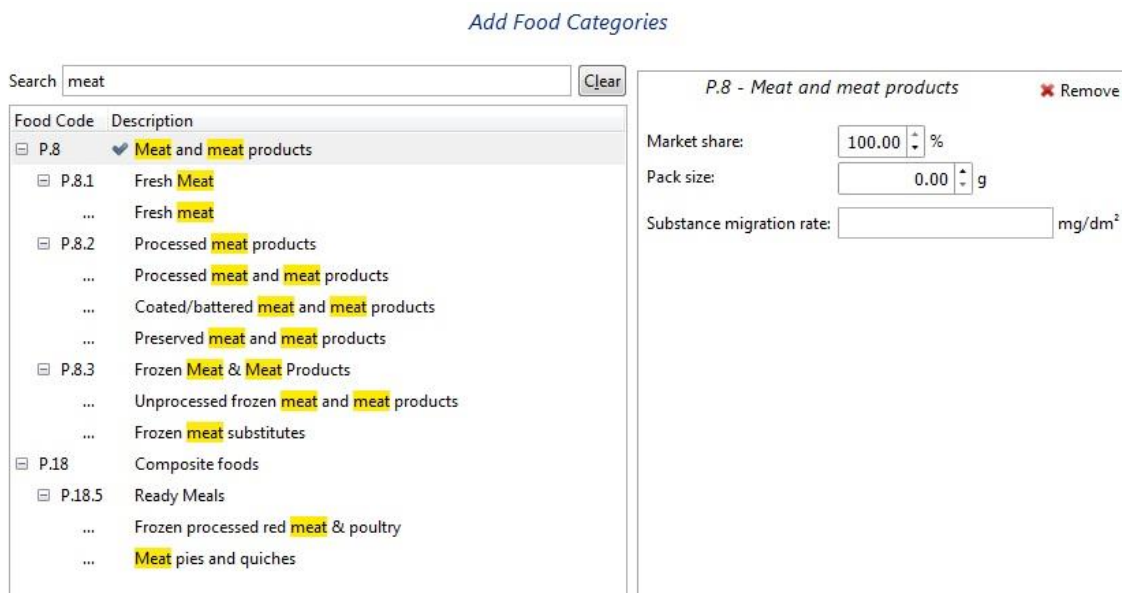


Figure 98: Create food category.

4. Table Options

This step presents you with a summary of the current choices of substances, populations and food categories for the assessment.

After reviewing the choices, you can choose to start an assessment using the “Submit” button at the bottom right of the window.

Equally, you may wish to make changes to the selections. Navigation to the appropriate steps to do this is easily achieved with the buttons on the left of the tab.

Table Options

Output file: /Data/My Data/My Migration Data/New Migration Data Table

Packaging type: NewMetalPackType
Substance type: Existing Substance
Substance code: 1334
Substance name: Styrene

Component	Type	Layers
Main	Aerosol can	1

Food categories:

Food Code	Description
P.8	Meat and meat products

Figure 99: Table Options

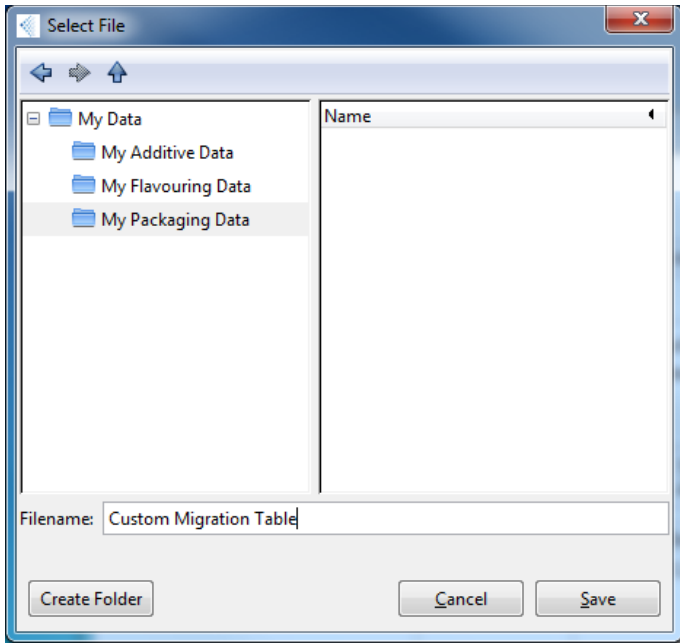


Figure 100: Saving custom migration to a file.

Known Issues

FACET 2.0.6 is prototype software and some minor issues may still exist. Please note that these issues will be eliminated in the final version of the software. In particular, the following issues have been recorded:

- Windows are known to freeze in certain cases. If this happens, follow the steps in the troubleshooting section on restarting the software.
- Opening and closing the same assessment repeatedly can cause FACET to crash.

Troubleshooting

Every effort has been made to ensure that FACET 2.0.6 is stable and error free. However, as the software is a prototype, some unforeseen issues may arise.

If the software stops working for some unknown reason, it is recommended that the following procedures be followed in sequence.

Restart the software

1. Close the software by clicking on the X in the top right corner of the main FACET window, or by selecting File and Exit. If this fails to close the program, proceed to the section called “Close FACET using the Task Manager”.
2. If FACET closes successfully, restart FACET by selecting Start -> All Programs -> FACET -> FACET 2.0.6
3. If the issue is still unresolved, proceed to the section “Close FACET using the Task Manager”.

Close FACET using the Task Manager

1. Press Ctrl + Alt + Delete on your keyboard.
2. Click on “Start Task Manager”.
3. Click on the “Processes” tab.
4. In the “Image Name” column, click on any process that begins with “FACET” to highlight it (e.g. “FACET Database.exe”, “FACET Scheduler.exe”, “FACET.exe”, or “FACET Engine.exe”), and then click the “End Process” button.

5. Repeat this process until all of the processes whose names begin with "FACET" have been terminated.
6. Restart FACET as normal, by selecting Start -> All Programs -> FACET 2.0.6
7. If the issue is still unresolved, proceed to the section, "Reset FACET".

Uninstall and reinstall FACET

1. If all of the above fails to resolve the issue, it may be necessary to uninstall and reinstall FACET on your computer.
2. On Windows XP: Click on Start -> Settings -> Control Panel -> Add or Remove Programs
On Windows Vista: Click on Start -> Control Panel -> Programs and Features
On Windows 7: Click on Start -> Control Panel -> Uninstall a Program
In each case, you should see FACET 2.0.6 in the list of programs.
3. Click on FACET 2.0.6 and select "Uninstall" or "Remove". This will remove FACET 2.0.6 from your computer.
4. Using your web browser, go to www.cremesoftware.com/facet and follow the download and installation instructions for FACET 2.0.6 to create a fresh installation of FACET on your computer.

Failing all of the above

If none of the above successfully rectifies the issue, please contact facet@cremeglobal.com and outline the problem. Please mention the Operating System used and Service Pack (e.g. Windows XP SP2 etc.). This information can be found by pressing the Windows + Pause Break keys.