Targeted Risk Assessment

User Guide for the integrated tool TRAM

Version 3 update to version 3.1

June 2014

User Guide for the TRA integrated tool – TRAM, version 3.1

Contents

1. INTRODUCTION

This User Guide is to help the reader in operating the ECETOC TRA v3.1 integrated tool. This User Guide does not provide guidance on the technical basis for the TRA. For that the reader is referred to the ECETOC Technical Reports 107 and 114, together with the Addendum to 114, Technical Report 124. The ECETOC TRA v3.1 uses colour codes to mark the differences between data fields. For that reason it is recommended to obtain a multicolour print of this user guide.

Subsequent to the 2010 REACH registration the ECETOC TRA v2 was developed to account for exposure assessments needing to be refined based on the scientific basis described in the ECETOC Technical Report 107 and 114 (TR 107 and TR 114). ECETOC TRA v3 which implements many of the refinement options outlined in TR 107. The introduction of v3.1 of the TRA enables the exposures and risks associated with the infrequent consumer uses of substances to be better the addressed. The ECETOC TRA integrated tool offers the exposure and risk assessment for workers, consumers and the environment in one single tool, the so-called 'integrated' tool or ECETOC TRAM. In addition, the consumer assessment tool is available as a standalone version.

Manual and Batch Mode

The ECETOC TRAM can be operated in a manual and a batch mode. In the manual mode, assessments are performed and saved one-by-one. In the manual mode, one substance can be assessed with fifteen scenarios in one single run. The batch mode allows for serial assessments. Both modes are administered via the datasheet 'Interface'.

Data Entry

Data entry can occur via the Interface or via the datasheets of the ECETOC TRAM. Assessments in the batch mode require that data are entered into the datasheets prior to the assessment. In the batch mode up to 60 scenarios can be assessed per substance. In addition to the serial assessments, the batch mode allows for enhanced reporting or results and supports advanced environmental assessments. Alternatively, data entered in the 'Interface' may be stored to the datasheets (see chapter 3.2).

Standard and Refined Assessments

Standard assessments can be performed in the manual and the batch mode. Advanced assessments available in the manual mode include all refinements of worker assessments; generating customised subcategories for consumer assessments; and the use of specific Environmental Release Categories (SPERCs) for environmental assessments. These options are also available via the batch mode. In addition, the batch mode exclusively offers the possibility to enter data to refine the environmental fate modelling (partition coefficients between water and various sub-compartments, and degradation rate constants), to derive PNECs following the R16 Technical Guidance, and to generate customised emission assessments.

Working in EXCEL 2007

The ECETOC TRA has been developed in the 2003 version of EXCEL. So far, it was found that operating the integrated ECETOC TRA from the 2007 version of EXCEL differs from the 2003 version for a small number of operations. This is due to the altered structure of the menu setup of these higher versions of EXCEL. Some of the changes will be addressed in Chapter 2.1, 2.2 of this user guide.

2. STARTING / EXITING THE APPLICATION

2.1 Starting

To start the integrated TRA, extract the file "Integrated tool v3,1.zip" into one single folder using WinZip or any other program capable of extracting .zip-files. The folder will then look as displayed in Figure 1. To run the application, double click on the file "ecetocTRAM.xls". The tool will then start. Enable macros when asked in message box and allow for linking to the remaining eight files. They will then open automatically.

Figure 1: Extracted TRA folder.
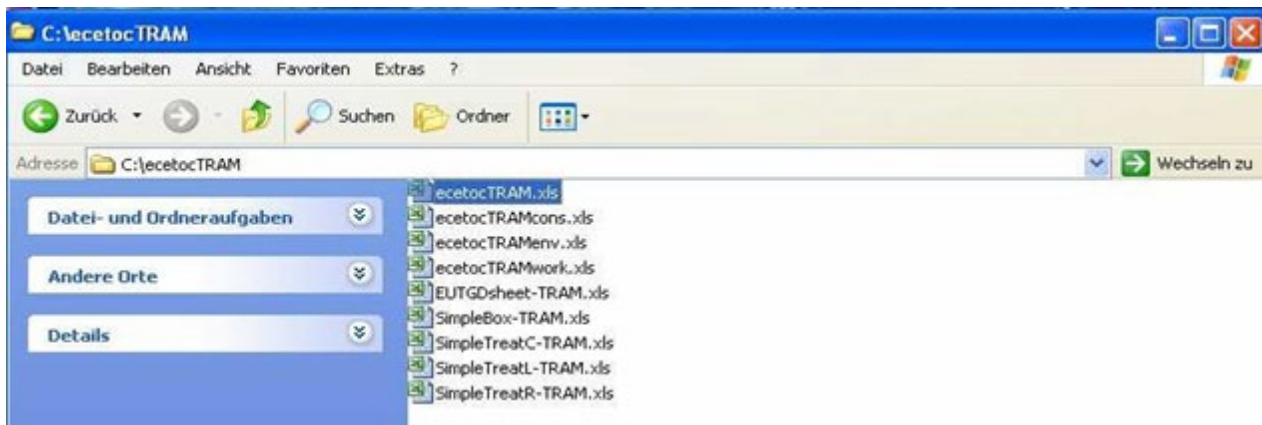
Extract the Integrated tool v3,1.zip into one folder and double-click on ecetocTRAM.xls to start the application. Enable macros when asked in message box. The remaining files will open automatically. Users of EXCEL 2007 are recommended to manually check all 9 files opened and to enable before entering data into the ecetocTRAM Interface spreadsheet.

Users of EXCEL 2007 and 2010 have to enable the macros in the ECETOC TRAM as shown below.
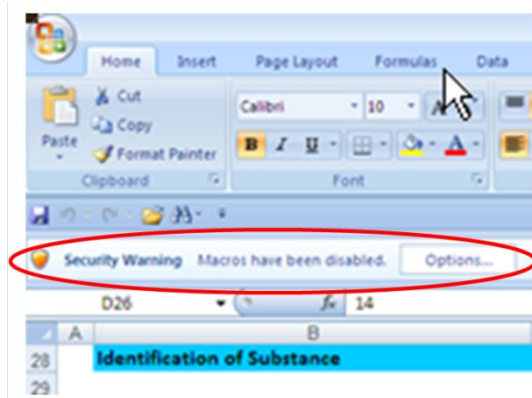
2.2 Exit the ECETOC TRA integrated tool

To save and leave the ECETOC TRA integrated tool and close all 9 files press Ctrl+e while the ecetocTRAM.xls is active. Alternatively, the button "ecetocTRAM" in the Excel command line may be used while the ecetocTRAM.xls is active which offers "Save and exit".

To leave the ECETOC TRA integrated tool and close all 9 files WITHOUT saving data, press Ctrl+t while the ecetocTRAM.xls is active.

Example for Excel 2003:
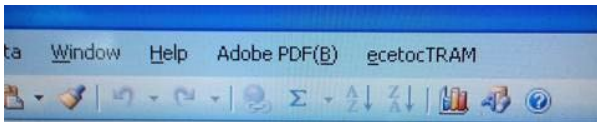
For Excel 2007/2010, the "Safe and exit" can be accessed via "Add-ins":
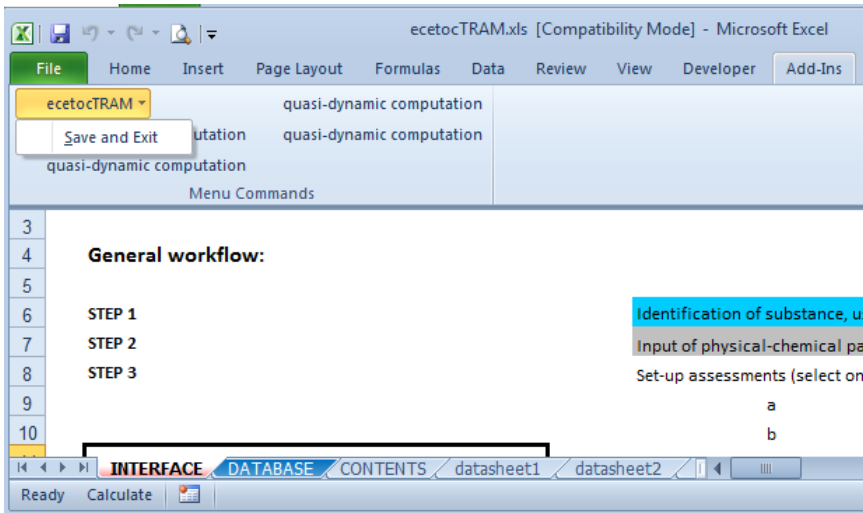
3. USER INTERFACE

3.1 Overview

The user interface allows for the exposure and risk assessment of a single substance in several uses for worker, consumer and the environment (maximum 15 scenarios each). The environmental assessment is limited to ERC- and SpERC-based exposure estimates (TIER II estimates are possible via the datasheets and using the batch mode exclusively).

The user interface is structured in the following way:

I.   General workflow and assessment management, i.e. options for running assessments from the User Interface (manual mode), clearing entries from Interface, retrieval from and storage to the datasheets and batch processing of datasets in the datasheets
NEW features in version 3.1: export and import of data sets for single substances from/into datasheets

II.   Identification of substance

III.   General physico-chemical data entry

IV.   Data entry for worker assessment

V.   Data entry for consumer assessment

VI.   Data entry for environmental assessment

3.2 Part I - General Workflow, Retrieval and Storage from and to the Datasheets, and Batch Processing

Part I (Figure 2) gives a short overview of the general workflow for an assessment. A substance from the datasheets can be read into the user interface ("Read" button in cell E 21) or the entered data can be stored into the datasheets ("Save" button in cell E 24). The "Clear" button in cell "I 21" allows for clearing all input and output fields in the user interface. The user can select to run a manual assessment of one substance ("Run" button in cell E 22 or to run a batch process. For batch processes, all assessments for human health (worker and consumer) and environment can be performed using the "Run batch" button (in cell E 26) to calculate the exposure and risk for several substances as entered into the datasheets). Alternatively, assessments for human health or environment can be run separately by using the "Run batch – Human health" or "Run batch – Environment" button (both in cell E27). This may reflect the work process in companies or just speeds up the batch run if e.g. refinement of only one part is required.

New features included in version 3.1 are the options to export and import data sets for single substances from/into datasheets.

To export the parameters for a substance, select the substance from the drop-down list in cell I24 (this is equivalent to the list in the "Contents" sheet) and click on the macro "Export substance" to the right (cell J24/25). Click on "Delete" when prompted. The toll has now created an Excel file (Book <x>) with one sheet named "Import" containing the data (substance data and assessment parameters only – no results) of the selected substance in the structure of the TRAM datasheets. This can be saved under a name of your choice and used for sharing. This is also the file structure required for the import function (NOTE: do not re-name

the sheet "Import" as this is needed for the import function).

To import substance data (from suitable files), click on the macro "Import substance" (cell I22/23), select the Excel source file to import the data (browse directories as usual, if needed) and click "Open". Click "Continue" when prompted and "No" in next Window popping up. The TRAM identifies the first available area/substance in the Datasheets for saving the substance information imported by checking for the substance name to be "empty" in the datasheets row 8, columns C, BL, etc. (compare "Safe" function further down in this chapter).

Figure 2: Overview of Part I of the user interface.

Yellow fields are data entry fields at the top of Part I. The new export/import features are placed on the right side of the UserInterface sheet.

Colour Codes for Input Fields

Input fields are marked with specific colours as indicated in cells H17 and H18. Yellow cells represent mandatory inputs, blue cells represent optional inputs. However in some cases (e.g. D44 – D48, partition coefficients) at least one of the blue fields needs to be filled. In addition, there are grey fields which do not accept input (or do not use any input that maybe made).

Indicator: Manual or Batch Mode

Cell D18 indicates whether one operates in manual ("m") or batch mode ("b"). This is not an entry field, but automatically set by the TRAM if an assessment of one substance is run from the user interface ("Run" button in cell E22) or a batch process is used ("Run batch" buttons in cell E26 or E27).

Entering Data into the User Interface for Manual Mode Assessment

How to enter the relevant data into the user interface for a manual calculation or for saving them to the datasheets is explained further down for Parts II – VI. The "Clear" button can be used to clear any existing

entries in the user interface in order to avoid confusion.

Run: Single Substance Assessment from User Interface in Manual Mode

To run the entered scenarios for the selected substance in the user interface, one simply needs to click on the "Run" button in cell E 22. All input data in the user interface are then transferred to the respective calculation tools (consumer, worker, and environment) and are processed. Afterwards the results are written back into the user interface into the results cells next to the input cells of each scenario (scroll right in each scenario line in the "Interface" to view results).

Save: Store Single Substance Assessment Data from User Interface to Datasheets

To save a substance just entered into the "Interface" into the "datasheets" click on "Save" (cell E24). All data visible in the user interface are then transferred into one of the datasheets (datasheet1-datasheets20) at the position indicated in cell D24. Datasheet1 contains substances 1 to 4, datasheet2 contains substances 5-8, and so on.

Practical note: The TRAM identifies the first available area/substance in the Datasheets for saving the substance information entered in the user interface by checking for the substance name to be "empty" in the datasheets row 8, columns C, BL, etc. You may use a substance number that had been populated before in the Datasheet by entering "empty" as the substance name. Check whether the TRAM has identified the substance number in D24 of the Interface and you can save the dataset from the Interface to this substance in the Datasheet.

Read: Retrieve Assessment Data from Datasheets into User Interface from Manual Run

In manual mode, one can read a substance with its scenarios from the datasheets by selecting a substance from the drop-down menu in cell D21 and then clicking on "Read" in cell E21. The data entered into the datasheets for this substance are then transferred to the interface.

Practical note: Only the first 15 worker and consumer scenarios will be read into the user interface (limitation of the user interface) and only ERC and SpERC inputs for environmental assessments will be transferred (no TIER II assessments). ERC and SpERC assessments will be assigned in G114-G128 in the Interface, but any TIER II assessments will be blank as they cannot be operated from the Interface. Please note that also the specification of the environmental assessment needs to be re-entered in column G because TIER II selection cannot be reflected in the INTERFACE.

Clear: Delete Entries of Single Substance from User Interface

To clear all entries of a substance in the "Interface" click on "Clear" (cell I21). All data visible in the user interface are then removed. The cells G114-G128 set to the default assessment (ERC) and the type of reference value per default set to PNEC or DNEL (for environment only).

Practical note: The combination of the "Clear" and "Safe" function can be used to remove datasets from Datasheets to create a blank sheet for new entries.

Batch Mode

When processing data in the batch mode, one needs to enter the starting substance number into cell I26 and the last substance to be processed into cell K26 of the interface. The substance number is the number under

which a substance is stored in the datasheets. The sheet "contents" gives an overview which substances are stored in the data base and where.

By clicking "Run batch" in cell E26, the tool starts to calculate all scenarios entered into the datasheets for the selected substances. Alternatively, assessments for human health or environment can be run separately by using the "Run batch – Human health" or "Run batch – Environment" (in cell E27).

Standard vs Advanced

Cell I27 allows the user to select "Standard" or "Advanced" form of the Batch mode. This only applies to environmental assessments. Using the advanced mode, more detailed results for the environmental assessment will be shown (e.g. PECregional) - compare output list on datasheets line 517 and below. It is also required to derive PNEC by the model based on ecotoxicological data inputs in the datasheets (line 188).

Practical note: A single substance can be run by entering the substance number in both cell I26 and K26. The results of the batch mode runs will be displayed in the respective area of the datasheet from row 444 onwards (assessed scenarios by column). Selective assessment of e.g. substance 1, 5, 9, etc. in batch mode is not possible.

3.3 Part II - Identification of substance

Part II (Figure 3) asks the user to enter required data for the identification of the substance to be assessed, like substance name and CAS number.

*Figure 3: Part II. Identification of substance.*
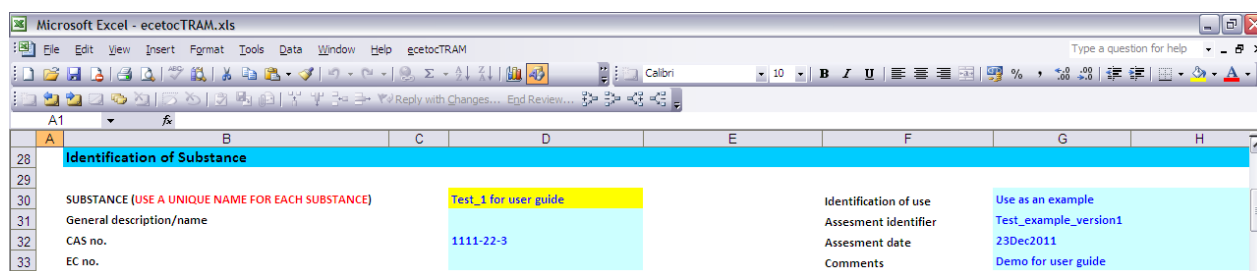
Cell D30 (SUBSTANCE) is a mandatory input. Here, enter the substance name under which the substance will be saved in the datasheets. The name needs to be unique. Cell D32 is for entering the CAS-No. of the substance. This field is also mandatory. All other cells in this section are optional entries: general name of the substance, CAS-No., EC-No., identification of use, assessment identifier, assessment date and comments. PCs, PROCs, ACs are entered in the respective human health parts further down, because they directly determine the assessed scenarios.

3.4 Part III - General physico-chemical data entry

Part III (Figure 4) is the screen for entering general physico-chemical data of the substance to be assessed.

Some data need to be entered as numbers (e.g. molecular weight, vapour pressure), some others need to be selected from a drop-down menu, like physical form. The fields displayed in blue are optional entries, but at least one of the optional fields needs to be filled in. Some fields (Partition coefficient octanol-water and Koc) offer the selection of entering either the value for Kow (cell D42) and Koc (D45) or their log units, which has to be specified by the user in cells E42 and E45 respectively. Also for the vapour pressure (cell D40) the user can select to enter the value in Pa or hPa (cell E40).

Figure 4: Part III. General physico-chemical data.
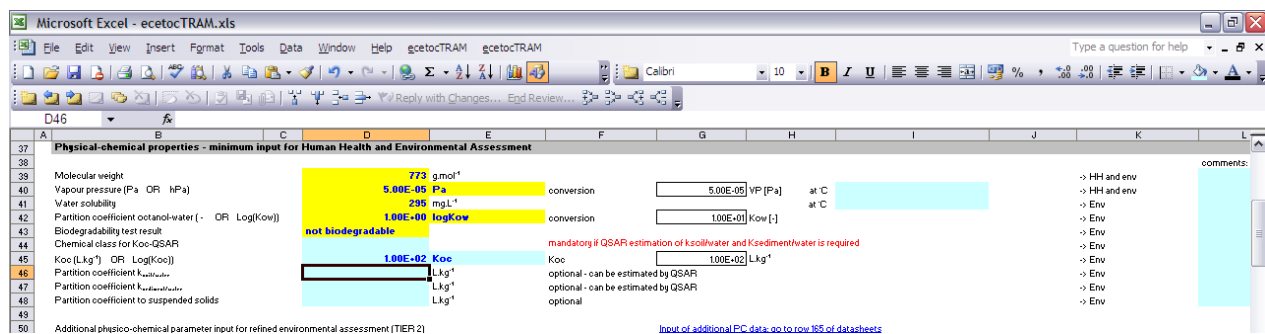
Lines 39 to 48 cover the entries of substance specific data which are of general relevance for the exposure assessment. Most fields require the entry of a number. These fields are: molecular weight, vapour pressure, water solubility and the relevant partition coefficients. Some fields require an input by selection of one option of the drop-down menus. These fields are: Biodegradability test result, Chemical class for KOC QSAR and Physical form. Special fields are Kow, Koc and Vapour pressure: besides entering a value, the type of value needs to be selected from a drop-down menu (Kow or logKow, Koc or logK$_{OC}$, Pa or hPa). The fields displayed in blue are optional inputs, however one of the options must be used, either a chemical class forKoc-QSAR has to be selected or at least one partition coefficient has to be entered.

Column K indicates where the parameters are used and comments e.g. on the source of the data can be recorded in column L.

Cell G50 (Input for additional PC data) states that additional PC data (e.g. various solid-water partition coefficients, rate constants for various degradation reactions) can be entered, if a refinement for some reasons will be necessary. Those additional data cannot be entered via the user interface. They have to be entered directly into the datasheets in lines 164-181.

3.5 Part IV - Data Entry - Worker Assessment

Part IV (Figure 5) shows the entry fields for worker exposure and risk assessment. Fifteen different uses can be entered here (lines 55 to 69), each with its own combination of PROC (D55-D69), operating conditions and exposure modifying factors. The glossary for PROCs can be found in line 72 or in the ECHA guidance R12. The entries to all fields, except the optional scenario name (B55-B69), which is a free text field, need to be done via a selection from drop-down menus (except a numerical value for vapour pressure in case of an

assessment for volatile substances at elevated process temperature in column G). Further down in this section there is an option to enter indicative reference values (D76 or H76 and D77), which can be DNELs or any other reference value. TRA version 3 includes also reference values for short-term inhalation and long-term dermal local exposure (H78 and D79). In column "Basis of reference value" (F76-F79) it should be stated which reference value is entered (e.g. DNEL, OEL, etc.). For more details on the single parameters please refer to the ECETOC Technical Reports (TR) 93 and 107 and 114.

Figure 5: Part IV. Worker exposure entry fields.

Lines 55 to 69 represent the input and output cells of the worker exposure and risk scenarios. In each line, one PROC can be selected from a drop down menu. A descriptive text can be assigned as a scenario name. Under "type of setting" the user needs to select whether the task is operated within a professional or an industrial setting. Whether the physical form during the process is solid or not can selected from a drop-down menu, also the dustiness in case it is a solid and the vapour pressure at operating temperature in case it is not a solid. The duration of activity, the use of local exhaust or/and general building ventilation (or if the operation takes place outdoors), the use of respiratory and dermal protection including efficiency and if the substance is used in a preparation (including percentage can be addressed via drop-downs. In column M, the assessor can set the assessment to consider the effect of local exhaust ventilation on dermal exposure.

Lines 76 to 79 represent entry fields for reference values, against which the calculated exposure will be compared. This can be DNELs or OELs or other reference value (preferably mg*m-3 for inhalation exposure, mg-1* kg-1*d-1 for (systemic) dermal exposure and µg * cm-2 for local dermal exposure). The type of value may be specified in the field "basis for reference value".

Practical note: TRAM version 3 offers the option to do a first estimate for short-term inhalation exposure and the related short-term DNEL inhalation can be entered here as well. Same applies to a long-term local dermal exposure assessment.

3.6 Part V - Data Entry - Consumer Assessment

Working with existing categories and sub-categories

Part V (Figure 6-1) covers the entries which specifically relate to consumer exposure and risk assessment. Up

to fifteen different scenarios can be entered into the drop-down menu fields and free-text fields (lines 83-97). The scenario name (B83-B97) can again be entered as free text. Cells D83-D97 are used for the selection of PCs or ACs from a drop-down list. This drop-down list is structured to start with PCs and then ACs that are covered by the TRA with default values and allow TIER I assessments for sentinel products or articles or specific sub-categories, if selected. The glossary for PCs and ACs can be found in lines 100 and 101 or in the ECHA guidance R12.

Further down in the drop-down list, all other PCs and ACs are available for the creation of new subcategories (see below for more information on new sub-categories).

In E83-E97 one can optionally select a product or article subcategory for refinement. The drop-downs allow the selection of subcategories depending on the PC or AC selected in column D of the same row. For more details on the subcategories please refer to ECETOC Technical Report 93, 107, 114, together with the Addendum to 114, Technical Report 124. In column F it may be selectable if the product is a spray. However there are some categories which can never be a spray or are always a spray. The drop-down is therefore only active to select "yes" or "no" where applicable. For more details on this topic see the consumer tool guidance and the report.

The remaining input cells in this section ("amount of product used per application", product ingredient fraction by weight", "skin surface area dermal and oral" are optional inputs. If nothing is specified here, default values will be used. For more details on the scientific issues and the meaning of the input fields and default values, please refer to the ECETOC Technical Report 93, 107 and the amendment to TR 107 (in preparation)..

Further down in this section (cells D105-D107) there is an option to enter indicative reference values, which can be DNELs or any other reference value. In column "Basis of reference value" (F105-F107) it can be stated which reference value is entered (e.g. DNEL, OEL, …). A special feature here is in cells D105 and H105, where the inhalation reference value can be specified in different dimensions (either $mg* \, m^{-3}$ or $mg*kg^{-1}*d^{-1}$).

Figure 6-1: Overview of the consumer input cells in the "Interface" sheet.

Each row represents one (contributing) consumer scenario. Scenario names can be entered in column B, PC and AC categories and their related sub-categories in column D and E, respectively. Further parameters are in columns F-L. Glossary for PCs and AC are in lines 100 and 102 (just for reference – no model inputs here!). Reference values (e.g. DNELs for consumers can be entered in rows 105-107.For new subcategories: Navigation button in cell D98. Row 92 shoes an example of a new sub-category selected for assessment with the entry cells for model parameters labeled to prevent user from entering data here. Column C also provides the information that data need to be edited in the sub-module (navigate via button in cell D98).

Practical note: Reference values for consumers entered in this section are used in the environmental assessment to compare with oral and inhalation exposure of man via the environment.

Creating New Sub-Categories

Working with new sub-categories

Columns D and E are set up to select new subcategories defined by the user and calculate the results in the assessment as for the existing TRA sub-categories (i.e. one or more of the rows in the user interface maybe a new subcategories while other are existing ones.). It is the intention that information available from the activity coordinated by DUCC (DUCC SCED Guidance) and intended to generate Specific Consumer Exposure Determinants (SCEDs) for common uses of consumer products is referred to at this stage. Before they can be used in the assessment by simple selection in columns D and E, they need to be created and populated by the user. To do this, click on the button "Create or edit new subcategory" in cell D98 (See Figure 6-1) and a macro will take the user to respective work area in the consumer sub-module (sheet "Add Subcategories"). In the sheet "Add Subcategories", a second macro can be activated by clicking on the button "CLICK TO ADD ROWS" next to cell B2 (Figure 6-2). The user will be asked how many rows (i.e. new sub-categories) shall be added. Please note that rows cannot be removed any more once they have been added.

Once the model parameters have been entered (see paragraph below), the new sun-category/ies need to be added to the drop-down for selection in the TRA by pushing the button "Finish new subcategories" (next to cell D2). The user will be taken back to the "ecetocTRAM" master file and can run the assessments for both existing and new sub-categories from the "Interface" (and in batch mode from the "datasheets" – see

section on batch mode below).

Practical note: Please note that the entry fields for model parameters in the TRA; ("Interface" and "datasheets") will be displayed in different format and the user will receive a respective warning message if a new sub-category was selected in order to advise that the parameters for new sub-categories cannot be edited in the user interface and datasheets but only in the consumer sub-module. Use macro to navigate to the consumer sub-module and edit existing new sub-categories.

Parameters for new sub-categories in the consumer sub-module

Column B is the same drop-down as already known from cells D83-D97 of the "Interface" for the selection of all PCs or ACs. In column D, the names of the new sub-categories can be entered by the user. Please make sure to use unique names in order to avoid confusion in the look-up functions (may return incorrect results). Column C supports the user by indicating that a sub-category name was already used in the existing sub-categories by displaying a red exclamation mark (see comment in cell D6). So he just needs to ensure no duplication within column D of this sheet.

Columns F-G, K-N, Q-S and V-Y allow the entry of an advanced set of model parameters. Some of them are the same as used in the user interface before (e.g. column F: Product is a spray?; column K: Product Ingredient Fraction by Weight).

In general, the input area is structure to address:

- "Product is a spray?" and "Product is a solid?" for PCs in columns F and G
- Routes of exposure and differentiation for adults and children in columns H-J
- Product Ingredient Fraction by Weight in column K
- Frequency of use – for all routes in column L
- Dermal parameters in columns M and N (related contact area values returned in column O and P)
- Oral parameters in columns Q, R and S (related contact area values returned in column T and U)
- Inhalation parameters in columns V - Y
- User comments can be captured in column AB

For more details on the use of new subcategories please refer to the updated user guide for the consumer tool (version 3.1) and the ECETOC TRA technical report and the addenda to it.

Figure 6-2: General part of the input area for new sub-categories in the consumer sub-module, sheet "Add Subcategories".

	A	B	C	D	E	F	G	H	I	J	K	L
1												
2		CLICK TO ADD BLANK ROWS (Added rows cannot be deleted but can be edited)		Finish new subcategory/ies					ROUTES OF EXPOSURE		ALL	Use Frequency - ALL routes
3						Only for PC			c = child, a = adult LEAVE		Enter value <=1	
4		Select from drop down		Free Text					BLANK if exposure pathway not relevant			FreQ of Use
5				Product Subcategory		Product is a spray?	Product is a solid?				Product Ingredient Fraction by Weight	(>= 1 event(s)/day as value or events/year from
6		Descriptor		(! in column left indicates duplication of name)		(default is "No")	(default is "No")	Dermal	Oral	Inh		drop-down)
8	1	PC3_Air_care_products		PC3_new_SC_1		Yes				a	0.5	2
9	2	PC13_Fuels		PC13_new_SC_1		No		a		a	1	Frequent
10	3	PC24_Lubricants_greases_and_release_products		PC24_new_SC_1		No		a		a	1	Infrequent
11	4	PC35_Washing_and_cleaning_products_including_solvent_based_products		PC35_new_SC_1				a			0.3	Frequent
12	5	PC1_Adhesives_sealants		PC1_new_SC_1		No		a		a	1	Very infrequent
13	6	PC1_Adhesives_sealants		PC1_new_SC_2		No		a		a	1	Frequent
14	7	PC1_Adhesives_sealants		glues, hobby use1		No		a		a	0.3	Frequent
15	8	PC1_Adhesives_sealants		glues, DIY use1		No		a		a	0.3	Frequent
16	9	PC1_Adhesives_sealants		glue from spray1		Yes		a		a	0.3	Frequent
17	10	PC1_Adhesives_sealants		sealants1		No		a		a	0.3	Frequent

The button "CLICK TO ADD ROWS" is next to cell B2 - user will be asked how many rows (i.e. new sub-categories) shall be added. The button "Finish new subcategories" (next to cell D2) is required to add the recently created "New sub-categories" to the selection lists in the "ecetocTRAM.xls file for batch processing.

Figure 6-3: Dermal and oral part of the input area for new sub-categories in the consumer sub-module, sheet "Add Subcategories".

	M	N	O	P	Q	R	S	T	U
2	DERMAL				ORAL				
3			ADULT	CHILD				ADULT	CHILD
4	Default = 1 (100%)				Default = 1 (100%)				
5				Skin Contact Area (cm²)					
6	TF dermal	Select body part exposed	Skin Contact Area (cm²)		TF oral	Select surface area mouthed	AC5 subcat type for default assessment	Contact Area (cm²)	Contact Area (cm²)
8									
9	0.002	3: palm of one han	210.0						
10	0.1	4: inside hands / o	428.8						
11		5: hands	857.5						
12	0.1	1: fingertips	35.7						
13	0.1	1: fingertips	35.7						
14		1: fingertips	35.7						
15		4: inside hands / o	428.8						

For dermal exposure, the selection of two additional body parts ("two fingertips" and "palm of one hand") was included. Parameters in columns S are only applicable for AC5 when "5: default" was selected in column R. Column S fields will then turn from grey shading into active cells with entry options from drop-down.

Figure 6-4: Inhalation part of the input area for new sub-categories in the consumer sub-module, sheet "Add Subcategories".

New parameters are the "Place of use" and the specification of a Transfer Factor (TF) for inhalation.

NOTE: For using the "New sub-categories" created in the "Add-subcategories" sheet in the Consumer sub-module in the batch processing of the datasheets in ecetocTRAM.xls master file, it is required to add the recently created "New sub-categories" to the selection lists in the "ecetocTRAM.xls file by clicking the macro button "Finish new subcategories" on the "Add-subcategories" sheet. If one of the "New sub-categories" is then selected for batch processing in the datasheets, the respective entry fields in the datasheets are de-activated (no editing possible). All parameter setting can only be done in the "Add-subcategories" sheet.

3.7 Part VI - Data Entry for Environmental Assessment

Part VI (Figure 7) covers the entries for an environmental exposure and risk assessment. The input via the user interface (manual mode) offers the possibility to assess exposure using the environmental release classes (ERC) defined in ECHA guidance R16 or using some more refined specific environmental release classes (SpERC) as a first step.

For the environmental exposure assessment, up to 15 different uses (lines 114-128), each characterised by a combination of life cycle stage, tonnage, ERC as the use descriptor related to environment (column H) and a fraction of the tonnage considered for a regional assessment, can be considered. The scenario name (B114-B128) is an optional free text field; the entry of the life cycle stage is also optional and several life cycles can be selected from a drop-down menu (D114-D128). The annual EU tonnage needs to be entered as a number. In cells E114-E128 the fraction of the tonnage considered for a regional assessment is selected via a drop-down menu. For more information on regional assessments please refer to the TRA report and the ECHA guidance Part D and R16. In cells G114-G128 the user needs to select whether he wants to use an ERC or a SpERC as a determinant for the exposure assessment. If ERC is selected here, column I of the environment section need to be filled to specify if there is a sewage treatment plant considered for this ERC (column I). A glossary for the ERCs can be found in line 131 and the ECHA guidance document R16. If 'SpERC' is selected as emission assessment method in column G, the organisation/industry sector for which the SpERC is relevant is selected in column J. In column K the particular SPERC is selected for the assessment. All SpERCs are based on the assumption that a municipal STP is available for wastewater treatment. Hence, for SPERC assessments column I can be left empty.

Amounts Used

For specifying 'Daily amount used at site [kg/d] for SpERC assessment' (column L) for point sources several scenarios are possible:

- the emission assessment is based on an ERC: the cell in column L is grey and no entry is possible. The 'Daily amount used at site [kg/d] for SpERC assessment is derived based on Chapter R16 of the ECHA Guidance.
- the emission assessment is based on a SPERC for which no value of M_{SPERC} is specified: the cell in column L is yellow. A value must be entered.
- the emission assessment is based on a SPERC for which a value of M_{SPERC} is been specified: the cell in column L is light blue. The value of M_{SPERC} displayed in column N. It can be overwritten by entering a value into column L.

For specifying 'Daily amount used at site [kg/d] for SpERC assessment' (column L) for wide dispersive uses the emission assessment the cell in column L is grey and no entry is possible, irrespective of ERC or SPERC emission assessment.

The above options for specifying 'Daily amount used at site [kg/d] for SpERC assessment' are analogous to the approaches taken in ECHA's CHESAR.

For more information about SpERCs please refer to the CEFIC SPERC Guidance and the ECETOC Technical 107 and the available SpERC Factsheets (SpERC Factsheets) Further down (cells D135- D141), the reference values for the different endpoints need to be entered for a risk characterisation as well as the indication which reference value it is (e.g. PNEC).

Practical note: ERC is a mandatory entry even if the assessment may be based on SpERCs or higher TIER approaches as it will define whether the assessment refers to a point source or a wide dispersive use.

For a higher TIER assessment the user is advised to enter the data directly into the datasheets (see batch mode). For details on the release estimation options see section 4, datasheets, the ECETOC Technical Reports 107 and TR114

Figure 7 : Part VI. Environmental exposure assessment input.
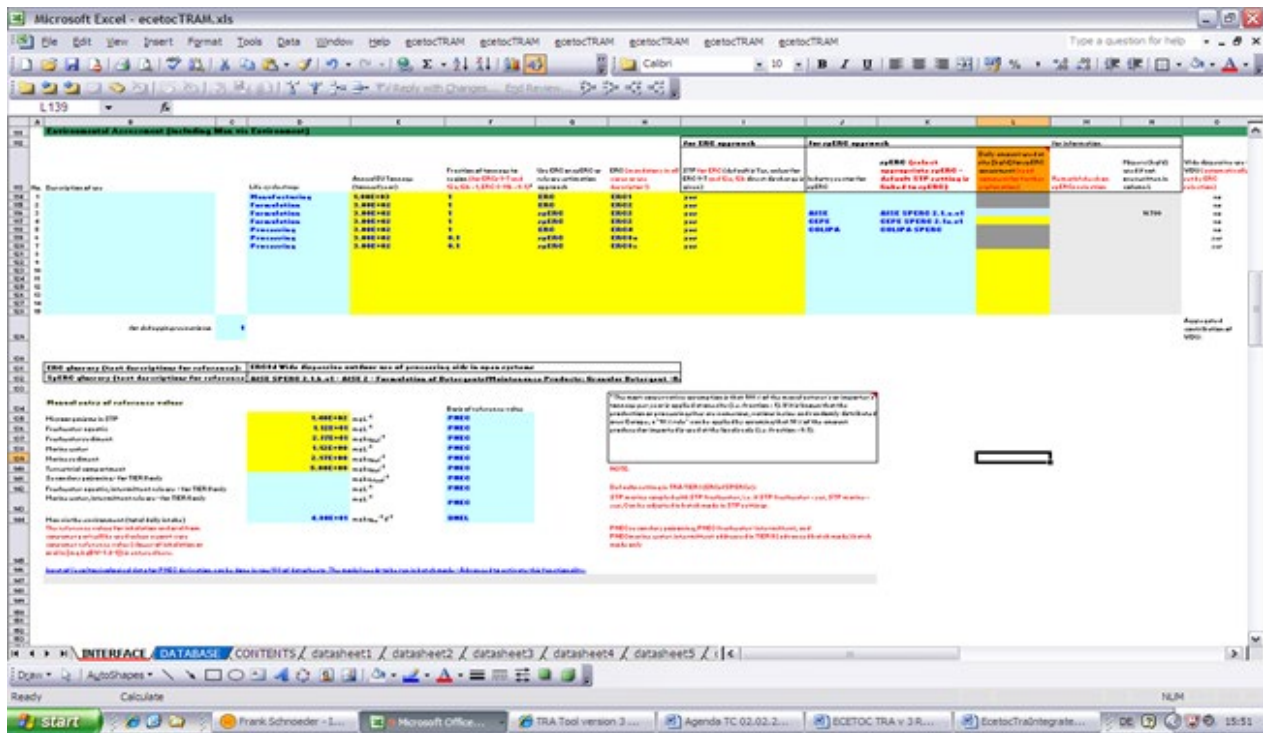
The environmental input is also set up in the same way as the human health input fields. There is an optional free text entry field for a descriptive use name and a drop down field for the selection of a life cycle stage. The annual EU tonnage is entered per life cycle stage, also the fraction of this tonnage that goes into the region. Here a value of 1 (100%) or 0.1 (10%) can be selected in line with the ECHA guidance document R16. The other columns allow for choosing between calculating the PECs based on the ERCs or SpERCs (specific ERCs). The entry in column "Use ERC or SpERC…" determines which approach will be used for the calculation, in column "ERC", the corresponding ERC for this use has to be selected (as use descriptor and for calculation of aggregated WDU, with or without STP in column "STP".

Alternatively, if SpERC is selected, the industry sector or sector organisation can be selected in column "Industry sector for SpERC", which provided SpERCs to the ECETOC TRA. In the last input column the corresponding SpERC can then be selected (column J and K).

Notes:
Column L allows the entry of the daily amount used at a site (in kg/d)where applicable and needed – see further details in Figure 7-2.

Column H will show a warning if the selected SpERC does not correspond to the ERC selected (check against the specification of the underlying ERC refined by the selected SpERC).

Practical note: Reference values for the assessment of exposure of 'man via the environment' have to be entered in the consumer section to compare with the predicted oral and inhalation exposure.

Figure 7-1: Part VI. Environmental exposure assessment input – General and ERC input.

Life cycle stage	Annual EU Tonnage (tonnes/year)	Fraction of tonnage to region (for ERCs 1-7 and 12a,12b = 1, ERC 8-11b = 0.1)*	Use ERC or spERC as release estimation approach	ERC (mandatory in all cases as use descriptor !)	for ERC approach OF STP for ERC (default is Yes, unless for ERC 1-7 and 12a, 12b direct discharge is given)
Manufacturing	1.00E+03	1	ERC	ERC1	yes
Formulation	3.00E+02	1	ERC	ERC2	yes
Formulation	3.00E+02	1	spERC	ERC2	yes
Formulation	3.00E+02	1	spERC	ERC2	yes
Processing	3.00E+02	1	ERC	ERC4	yes
Processing	3.00E+02	0.1	spERC	ERC8a	yes
Processing	3.00E+02	0.1	spERC	ERC8c	yes

Figure 7-2: Part VI. Environmental exposure assessment input – SpERC related input.

for spERC approach		Daily amount used at site [kg/d] for spERC assessment (read comment for further explanation)	for information		Wide dispersive use - WDU (automatically set by ERC selection)
Industry sector for spERC	spERC (select appropriate spERC - default STP setting is linked to spERC)		Remark/check on spERCs selection	Msperc (kg/d) used if not overwritten in column L	
					no
					no
AISE	AISE SPERC 2.1.a.v1			16700	no
CEPE	CEPE SPERC 2.1a.v1				no
					no
CEPE	CEPE SPERC 8a.n.v1				yes
					yes
CEPE	CEPE SPERC 5.na.v1		Check spERC vs. ERC!		no

The daily amount used at a site (kg/d) may be entered for point source assessments. If there is no M_{SPERC} defined, the cell is formatted in yellow indicating a mandatory input (example CEPE SPERC 2.1a.v1). If a M_{SPERC} is defined, the cell is formatted in blue indicating an optional input (example AISE SPERC 2.1a.v1 - M_{SPERC} is 16700 kg/d). If ERCs or SpERCs for wide dispersive uses are selected, the cell is formatted in grey – no entry should be done (will be ignored!)

Note: The last SpERC selected was not a refinement of the selected ERC (use descriptor) and the warning message alerts the user to check for consistency.

Figure 7-3: Part VI. Environmental exposure assessment input – Reference value input.

Manual entry of reference values

			Basis of reference value
Microorganisms in STP	1.40E+02	mg L^{-1}	PNEC
Freshwater aquatic	1.12E+01	mg L^{-1}	PNEC
Freshwater sediment	2.17E+01	mg kg$_{dwt}$$^{-1}$	PNEC
Marine water	1.12E+00	mg L^{-1}	PNEC
Marine sediment	2.17E+00	mg kg$_{dwt}$$^{-1}$	PNEC
Terrestrial compartment	5.00E+00	mg kg$_{dwt}$$^{-1}$	PNEC
Secondary poisoning - for TIER II only		mg kg$_{food}$$^{-1}$	PNEC
Freshwater aquatic, intermittent release - for TIER II only		mg L^{-1}	PNEC
Marine water, intermittent release - for TIER II only		mg L^{-1}	PNEC
Man via the environment (total daily intake)	4.80E+01	mg kg$_{bw}$$^{-1}$ d^{-1}	DNEL

The reference values for inhalation and oral from consumer part will be used unless a worst case consumer reference value (=lower of inhalation or oral in [mg.kgBW-1.d-1]) is entered here.

4. OUTPUT OF RESULTS IN THE USER INTERFACE

The output of the three parts "consumer", "worker" and "environment" exposure and risk assessment are structured in a similar way. The first columns always show the estimated exposure values, the following columns show the "risk characterisation ratios" (RCRs), the exposure divided by the reference value. If a risk is estimated for a use, the respective cell is highlighted in red (Figure 9).

The outputs are always arranged adjacent to the columns of the use inputs in the same line, so that one line always displays the input and the result for a specific use (e.g. line 55 is the first worker use with its PROC and conditions as input in cells D55-L55 and the corresponding results in O55-X55.

4.1 Output of the Worker Exposure and Risk

The output of the calculated exposures and RCRs for workers can be found in cells O54 to Z69. Column O covers the results for inhalative exposure in ppm, column P covers inhalative exposure in mg/m^3 and column Q dermal exposure in mg/kg/day. In TRA version 3 short-term inhalation in mg/m^3 (column R) and long-term dermal local exposure in µg/cm^2 (column S) were included in the assessment. If for a certain route (inhalative or dermal) no exposure can be estimated the result is #NV (Figure 8). Columns V to Z show the RCRs for the corresponding routes.

Figure 8: Worker output fields in the user interface

In the columns adjacent to the input fields, the respective results of the calculation are shown, after the "run" button was activated and the scenarios were calculated. Displayed is the calculated exposure for the different routes and the resulting risk characterisation ratio. Red fields indicate an RCR>1, green fields indicate an RCR<1.

Practical note: The total exposure for human health was removed from the report and only the total RCR is reported in version 3. However, important comments/remarks regarding the predicted exposure is now provided to the user in column R. Particularly the effectiveness of LEV for inhalation exposure (and dermal exposure, where applicable) is reported.

4.2 Output of the Consumer Exposure and Risk

The consumer results are structured in the same way as the worker results with one specialty: Columns N-V show the results calculated for the product subcategories (if a product or article subcategory was specified) and columns X-AF show the results calculated for the "sentinel" product categories (if no product or article sub-category was specified) (Figure 9). For details on subcategories and sentinel products please refer to the user guide for the consumer tool and the TRA report.

Figure 9-1: Consumer output fields for Product Subcategory in the user interface.

OUTPUT BY PRODUCT SUBCATEGORY

Inhalation exposure (mg.kg-1.d-1)	Dermal exposure (mg.kg-1.day-1)	Oral exposure (mg.kg-1.day-1)	Inhalation exposure (mg.m-3)		Risk Characterisation Ratio - Inhalation	Risk Characterisation Ratio - Dermal	Risk Characterisation Ratio - Oral	Risk Characterisation Ratio - Total
1.34E-01	0.00E+00		1.47E+00		1.34E-02	0.00E+00		1.34E-02
5.53E+00	0.00E+00		4.04E+01		5.53E-01	0.00E+00		5.53E-01
5.38E-01	0.00E+00		5.88E+00		5.38E-02	0.00E+00		5.38E-02
1.34E+00	0.00E+00		1.47E+01		1.34E-01	0.00E+00		1.34E-01
2.02E-01	1.78E+01	7.42E-01	2.21E+00		2.02E-02	1.78E+00	7.42E-01	1.88E+00

In the columns adjacent to the consumer input fields, the respective results of the calculation are shown, after the "run" button was activated and the scenarios were calculated. The calculated exposure for the different routes is displayed and the resulting risk characterisation ratio for the sub-categories. Red fields indicate an RCR>1, green fields indicate an RCR<1.

Note: Empty line may occur if no sub-category was specified and, thus, only results for sentinel products were calculated (see Figure 9-2).

Figure 9-2: Consumer output fields for Sentinel Products in the user interface.

OUTPUT BY SENTINEL PRODUCT CATEGORY

Inhalation exposure (mg.kg-1.d-1)	Oral exposure (mg.kg-1.day-1)	Inhalation exposure (mg.m-3)	Dermal exposure (mg.kg-1.day-1)	Risk Characterisation Ratio - Inhalation	Risk Characterisation Ratio - Dermal	Risk Characterisation Ratio - Oral	Risk Characterisation Ratio - Total Exposure
5.53E+00	2.14E+01	0.00E+00	4.04E+01	5.53E-01	2.14E+00	0.00E+00	2.70E+00
4.97E+00	5.95E-02	0.00E+00	8.70E+02	4.97E-01	5.95E-03	0.00E+00	5.03E-01
3.69E+00	1.29E+02	0.00E+00	4.04E+01	3.69E-01	1.29E+01	0.00E+00	1.32E+01
1.84E+00	1.43E+02	1.00E+01	4.04E+01	1.84E-01	1.43E+01	1.00E+00	1.55E+01
	1.27E+02	6.75E+01			1.27E+01	6.75E+00	1.95E+01
	7.15E+01	1.50E+01			7.15E+00	1.50E+00	8.65E+00
3.69E+00	7.15E+01	0.00E+00	4.04E+01	3.69E-01	7.15E+00	0.00E+00	7.51E+00
3.69E+00	7.15E+01	0.00E+00	4.04E+01	3.69E-01	7.15E+00	0.00E+00	7.51E+00
9.07E+01	7.15E+01	0.00E+00	9.93E+02	9.07E+00	7.15E+00	0.00E+00	1.62E+01
New subcat	New subcat	New subcat	New subcat	New subcat	New subcat	New subcat	New subcat
7.38E+00	1.03E+03	4.30E+00	4.04E+01	7.38E-01	1.03E+02	4.30E-01	1.04E+02
3.69E+00	1.46E+01	0.00E+00	4.04E+01	3.69E-01	1.46E+00	0.00E+00	1.83E+00
7.38E+00	5.57E+01	3.00E+00	4.04E+01	7.38E-01	5.57E+00	3.00E-01	6.61E+00
3.69E+00	3.47E+00	1.00E+00	4.04E+01	3.69E-01	3.47E-01	1.00E-01	8.16E-01
7.38E+00	6.27E+01	7.17E-01	4.04E+01	7.38E-01	6.27E+00	7.17E-02	7.08E+00

In the columns adjacent to the consumer input fields, the respective results of the calculation are shown, after the "run" button was activated and the scenarios were calculated. The calculated exposure for the different routes and the resulting risk characterisation ratio for the sentinel products. Red fields indicate an RCR>1, yellow fields indicate an RCR<1.

Note: No sentinel product results will be reported for NEW sub-categories created by the user (see example in row 10 above).

4.3 Output of the Environmental Exposure, Risk and Safe Amount for Handling (M$_{SAFE}$)

The consumer results are structured in the same way as the results for workers. There is one exception: Besides the exposure or predicted environmental concentrations (PECs) and the RCRs also the maximum amount for safe handling (M$_{SAFE}$) is shown in columns AA-AG (Figure 10). For details on this parameter please refer to the TRA report.

Figure 10: Environmental output fields in the user interface.

In the columns adjacent to the environmental input fields, the respective results of the calculation are shown, after the "run" button was activated and the scenarios were calculated. Displayed is the calculated exposure for the different routes, the resulting risk characterisation ratios and the maximum amount for safe handling. Red fields indicate an RCR>1, green fields indicate an RCR<1.

5. DATASHEETS

The datasheets consist of 20 tabs in the ecetocTRAM.xls called "datasheet1" to "datasheet20". Each datasheet offers the possibility to save four substances with up to 60 (contributing) scenarios for worker and consumer and up to 24 scenarios for environment. In total up to 80 substances, with up to 60 uses for consumer and worker and 24 for environment, can be saved in the datasheets. Substances can be saved there via the save button in the user interface (limited to 15 uses) or by direct entry into the datasheets. Entering data directly into the datasheets is for advanced users and offers also the possibility to enter data which might become necessary for a refinement. The datasheets offer the possibility to enter more detailed physico-chemical data, environmental fate data and (eco)toxicological data for deriving PNECs.

5.1 Datasheets – Entering Input for Standard Assessments

The upper part of the datasheets is structured in a similar way as the user interface (Figure 11). The first part is the identification of substance, followed by the basic physico-chemical data. The next parts cover up to 60 scenarios for worker, consumer and 24 for the environment. In contrary to the user interface one use is not arranged in one line but in one column (e.g. cells D34-D42 covers the input parameters for the first worker scenario per datasheet).

Column B of the datasheets contains the description of all possible input parameters of the TRA.

The datasheets interact with the user interface via the "read" and "save" buttons. Since the user interface does not cover all cells which can be filled in the datasheets, only those reflected in the user interface can be read via the "read" button and be saved via the "save" button (i.e. worker scenarios 1-15, consumer scenarios 1-15 and environmental scenarios 1-15) .

Figure 11-1: Upper part of a datasheet with worker inputs.

Column B contains the description of all possible input and output parameters. The structure of the upper part equals the structure of the user interface. One use is represented in one column (red ellipse). Yellow fields are mandatory inputs for exposure parameters, blue fields are optional, as in the user interface. Reference values in column C have been extended to short-term inhalation (15 minutes average) and long-tern local dermal in TRA v3.1.

In total the ecetocTRAM.xls offers 20 datasheets to cover 80 substances with up to 60 (contributing) scenarios for worker and consumer and 24 for the environment.

For the consumer assessment part, the same parameters as used in the "Interface" sheets are available, but in columns instead of rows (same as for worker assessments). The button to navigate to the consumer sub-module to create or edit new sub-categories is located in column B (cell B53).

Figure 11-2: Consumer input part of a datasheet.

One use is represented in one column (pink ellipse). Yellow fields are mandatory inputs, blue fields are optional, as in the user interface. Button to navigate to the consumer sub-module is in cell B53.

5.2 Datasheets – Entering Input for Advanced Assessments

Emission Assessment via Datasheet

All entries for refinement are formatted as "optional" (i.e. not required for ERC or SpERC based assessments), but are required for TIER II exposure assessments.

In the datasheets, the daily site amount for SpERCs may be entered in line 79, M_{SPERC} would be reported in line 89 and a related message in line 90 following the same logic as described for the Interface. For TIER II assessments, the daily site amount is entered in lines 123 and 130.

Where a daily site amount (Msite in kg/d) is entered (and this also applies to SpERCs, where applicable), Fmainsource is calculated as:

= Msite / (EU Tonnage * 1000 * Fregion/Temis) OR

= Msite / (Tregion * 1000 /Temis)

The selection of the release estimation method/approach for environmental assessments in the datasheets is done via 4 drop-down cells (lines 102, 103 and 105 106- Figure 12). Only one can be set to "TRUE" (warning message will appear in line 107 if more than 1 "TRUE" was selected).

Figure 12: Selection of the release estimation method for environmental assessments in the datasheets (TIER I and TIER II).

102	Select approach ERC		FALSE
103	Select approach spERC		TRUE
104	TIER II Assessment Approaches:		
105	Select approach using SPECIFIC RELEASE FRACTIONS		TRUE
106	Select appraoch using MEASURED DATA (releases in kg/day)		FALSE
107	**ECETOC TRA FLAT DATABASE - INPUT TIER 2**		only 1 TRUE
108	**Environmental Assessment (including Man via Environment)**		

The example shows the error message returned if two methods were set to "TRUE".

Refining Environmental Assessments beyond SPERCs

Lines 109-181 are for entering input parameters for a refined environmental assessment (Figures 13-1 and 13-2). In lines 116 the type of RMM is specified as free text. In line 117 the associated efficiency of the RMM is entered as numerical value (in %). Lines 121-127 can be used for entering release factors (e.g. from OECD ESDs), lines 130-138 for entering amounts release in [kg/day] derived e.g. from measured data.

Lines 141-146 cover specific data on sewage treatment plants. Line 143 offers the possibility to override the default specify that a sewage treatment plant treats wastewater which is discharged to the marine environment. In lines 165-173, refined physico-chemical data can be entered and in lines 176-181 degradation and transformation rates can be entered.

Practical note: TRAM version 3 reduced the TIER II inputs for release estimation to release fractions and release rates (in [kg/day]) and provides fields in lines 109-119 of the datasheets to explain/justify the TIER II parameters used for refinement.

Please note that the RMM efficiency (%) documented in this part will also be used in the generation of scaling parameters. Therefore, any combined RMMs can be described in free text in the RMM lines, but the resulting total efficiency needs to be entered in the efficiency lines.

If an ERC of SpERC based assessment is to be refined by additional RMMs, the release fractions can be picked from lines 153-155 of the original scenario assessed and entered into the TIER II section of the refined scenario (lines 125-127, e.g. by copy/paste special - values). The additional RMM efficiency can then be directly factored into the refined release fraction using the efficiencies specified in lines 115, 117 and/or 119 as follows:

Refined release fraction = original release fraction * (1-efficieny of RMM)

Example 2% release in ERC 2 to air to be refined via RMM efficiency in cell D115 (%):

Refined release fraction = 0.02 * (1-D115)

Figure 13-1: Optional input for a TIER II environment assessment with release estimates based on release fraction (displayed example, e.g. from OECD emission scenario documents) or release rates (e.g. from measured data – not populated in example).

102	Select approach ERC	FALSE
103	Select approach spERC	FALSE
104	TIER II Assessment Approaches:	
105	Select approach using SPECIFIC RELEASE FRACTIONS	TRUE
106	Select appraoch using MEASURED DATA (releases in kg/day)	FALSE
107	**ECETOC TRA FLAT DATABASE - INPUT TIER 2**	
108	**Environmental Assessment (including Man via Environment)**	
109	**Justifications for refined release parameters**	
110	Basis used for refinement (e.g. ERC, SPERC)	ERC
111	Fraction of EU tonnage to region (-) - modified in line 78	ERC default
112	Daily amount used at site [kg/d]	adjusted to reflect larges
113	Release times per year (d/year)	conservative number assu
114	Local release to air - RMM	ERC default
115	Local release to air - efficiency of RMM (%)	n/a
116	Local release to sewage - RMM (beyond STP)	Oil-water separation
117	Local release to sewage - efficiency of RMM (%)	90%
118	Local release to soil - RMM	ERC default
119	Local release to soil - efficiency of RMM (%)	n/a
120	**RELEASE ESTIMATION BASED ON SPECIFIC RELEASE FRACTIONS**	
121	Comments 1	only RMM for waste wate
122	Comments 2	STP and river flow = defa
123	Daily amount used at site [kg/d] (release fractions)	1000
124	Release times per year (d/year)	100
125	Local release fraction to air	0.05
126	Local release fraction to sewage	0.006
127	Local release fraction to soil	0.0001
128		
129	**RELEASE ESTIMATION BASED ON RELEASE RATES, e.g. measured data (releases in kg/day)**	
130	Daily amount used at site [kg/d] (release rates)	
131	Release times per year (d/year)	
132	Name of Monitoring Site or other source of information	
133	Remark	
134	Monitoring regime	
135	Remark	
136	Measured. Release to air (kg/d)	
137	Measured Release to sewage (kg/d)	
138	Measured Release to soil (kg/d)	
139		
140	**STP PARAMETERS (can be used to refine also ERCs and spERCs except for STP [yes/no])**	
141	Use of local STP (yes/no)	yes
142	Local STP with primary settler?	yes
143	Use STP local marine?	yes
144	SludgeToSoil? (yes/no)	yes
145	River flow (m3/d)	18000
146	Effluent discharge rate of local STP (m3/d)	2000

Refined Physical-Chemical and Degradation Data

Also some additional physical-chemical data and degradation rates can be entered for a refined assessment.

Figure 13-2: Optional input for a TIER II environment assessment with release estimates based on release fraction (e.g. from OECD emission scenario documents) or release rates (e.g. from measured data).

164	**PHYSICAL-CHEMICAL SUBSTANCE PROPERTIES**	
165	Vapour pressure at the temperature of the data set (Pa) - from TIER I	
166	Temperature at which vapour pressure was measured (degrees C)	25
167	Water solubility at the temperature of the data set (mg.l-1) - from TIER I	
168	Temperature at which solubility was measured (degrees C)	
169	Melting point (degrees C)	
170	Solids-water partition coefficient raw sewage sludge (l.kg-1)	
171	Solids-water partition coefficient settled sewage sludge (l.kg-1)	
172	Solids-water partition coefficient activated sewage sludge (l.kg-1)	
173	Solids-water partition coefficient effluent sewage sludge (l.kg-1)	
174		
175	*DEGRADATION AND TRANSFORMATION RATES*	
176	Rate constant for degradation in STP (d-1)	
177	Total rate constant for degradation in surface water at env. Temp (d-1)	
178	Total rate constant for degradation in marine water at env. Temp (d-1)	
179	Total rate constant for degradation in bulk sediment at env. Temp (d-1)	
180	Rate constant for degradation in air (d-1)	
181	Total rate constant for degradation in bulk soil at env. Temp (d-1)	0.005

Also some additional physical-chemical data and degradation rates can be entered for a refined assessment.

PNEC Derivation analogous to EUSES

Lines 183 – 441 offer the possibility to enter data for deriving the PNECs in the same way as it was done in the TGD-Excel spreadsheet version of EUSES (Figure 14). This option is only available in the "advanced" batch mode.

However, many users will have derived PNECs outside of the TRAM and will not use these rows. Therefore, a new feature was added to expand the related rows in the input and output by a macro button in line 183. To collapse the PNEC derivation area, a second button is available in line 186 (only visible in expanded mode). The "Expand" / "Collapse" function will also apply to the PNEC results area in the results section of the datasheets.

Figure 14: Optional input for PNEC derivation based on (eco)toxicological data.
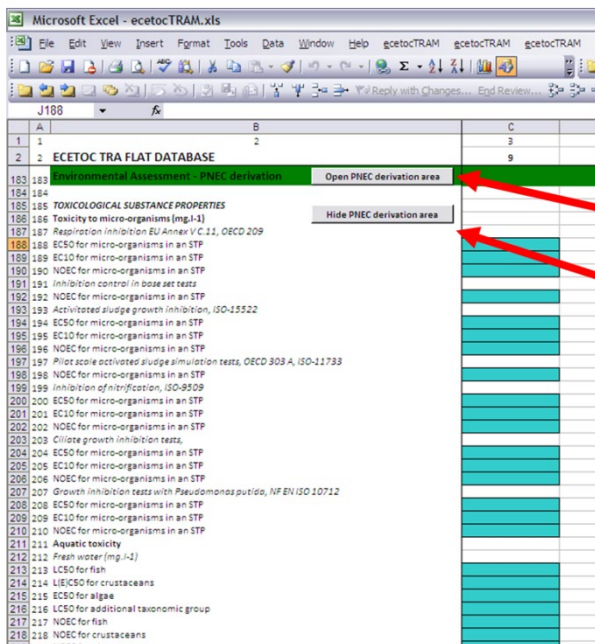
"Expand" button

"Collapse" button

The PNECs are derived the same way as within EUSES or the TGD Excel Spreadsheet model.

Practical note: Alert: Upon pushing the button 'Open PNEC derivation area' (line 183), the screen moves to the far left, i.e. the columns of the first substance in the respective datasheet. Hence, make sure to input the data into the correct substance (i.e. check that the inputs are made into the correct columns).

5.3 Output within the Datasheets

The output within the datasheets is structured in the same way as the input: worker, consumer, environment TIER I, followed by environment TIER II (Figure 15). Derived PNECs are displayed if the respective area was expanded by using the macro button in line 183 as described above.

As in the user interface the output is arrange in a way that it related directly to the input. The output in a certain column is the result of the estimation for the use put in the same column (output of column D is the result of the scenario put in column D).

Figure 15: Output of a worker assessment within the datasheets.

The output is structured in the same way as the input. The output of one column reflects the result of the estimation for a use put in the same column.

Interim Results of the Environmental Emission Assessment

Lines 151-162 display the results of the emission assessment (see Figure 16). The following information is specified per use: the amount used locally (line 151), the number of days at which emissions occur (line 152), the release fractions (lines 153-155, to air, water, and soil, respectively – these are the release fractions as stated in the ERC or SPERC background tables or set in line 125 of the Datasheet), and the local release rate (line 156-158, to air, water, and soil, respectively, - the release rates take into account that for wide dispersive uses, the local release will be considered 0 in accordance with the ECHA Guidance document R.16). Lines 159-161 specify the regional releases to air, water, and soil which are cumulated over all individual uses. These regional releases are used as input to the PEC$_{Regional}$ calculation.

Figure 16: Example output of Interim results for volumes and releases in environment assessments.

Additional output is generated by TRAM version 3.1 for the environmental assessments at the bottom end datasheets to correspond to the REACH Chemical Safety Report template (ECHA ES format).

Figure 17: Example output of additional assessment results for the environmental compartment for the REACH Chemical Safety Report template.

	A	B	BM	BN	BO	BP
1	1	2	65	66	67	68
2	2	ECETOC TRA FLAT DATABASE				
803	803	NEW ECHA CSR Template				
804	804	Local concentrations for MvE - oral route				
805	805	Drinking water	3.49E-02	5.22E-02	3.20E-04	
806	806	Fish	4.93E-02	7.37E-02	4.52E-04	
807	807	Leaf crops	8.86E-01	1.13E-03	6.17E-05	
808	808	Root crops	1.51E-02	8.99E-05	7.14E-05	
809	809	Meat	5.28E-05	2.35E-06	1.76E-08	
810	810	Milk	5.28E-04	2.35E-05	1.76E-07	
811						
812	812	Regional concentrations for MvE - oral route				
813	813	Drinking water	3.20E-04	3.20E-04	3.20E-04	
814	814	Fish	4.52E-04	4.52E-04	4.52E-04	
815	815	Leaf crops	6.15E-05	6.15E-05	6.15E-05	
816	816	Root crops	6.04E-05	6.04E-05	6.04E-05	
817	817	Meat	1.75E-08	1.75E-08	1.75E-08	
818	818	Milk	1.75E-07	1.75E-07	1.75E-07	
819						
820	820	Local contribution to oral route (dose)				
821	821	Drinking water	9.98E-04	1.49E-03	9.15E-06	
822	822	Fish	8.09E-05	1.21E-04	7.42E-07	
823	823	Leaf crops	1.52E-02	1.93E-05	1.06E-06	
824	824	Root crops	8.31E-05	4.93E-07	3.92E-07	
825	825	Meat	2.27E-07	1.01E-08	7.55E-11	
826	826	Milk	4.23E-06	1.88E-07	1.41E-09	
827						
828	828	Regional contribution to oral route (dose)				
829	829	Drinking water	9.15E-06	9.15E-06	9.15E-06	
830	830	Fish	7.42E-07	7.42E-07	7.42E-07	
831	831	Leaf crops	1.05E-06	1.05E-06	1.05E-06	
832	832	Root crops	3.32E-07	3.32E-07	3.32E-07	
833	833	Meat	7.54E-11	7.54E-11	7.54E-11	
834	834	Milk	1.41E-09	1.41E-09	1.41E-09	

Scaling Parameters for Environmental Scenarios Assessed

A new output section was added to the TRAMv3 environmental results in order to support the generation of data required for scaling. These results are only provided in the "advanced" batch mode (i.e. via "Run batch" or "Run batch – Environment" in the INTERFACE with Cell I27 set to "Advanced") and are displayed in lines760 and below (see Figure 17). As for the PNEC derivation, a macro button is available in line 760 to expand this area with the scaling results and a second macro button to collapse it. Two sets of data are generated per environmental scenarios related to point sources (NOT for wide dispersive uses) and directly feed into scaling tools, e.g. the GEST tool (in preparation). For other scaling tools using these parameters, the order/format/etc. may need to be adjusted for input.

Practical note: After running a manual run via the user interface results are not automatically saved in the datasheets. For saving the results of a manual run via the user interface the save button has to be activated to save the results and the input parameters to the datasheets (see "Safe" function in Part 1 of this user guide).

Figure 18: Example output of scaling parameters for environment feeding into a "simple scaling tool" / DU ES Conformity tool as currently developed.

	A	B	BM	BN	BO
1	1	2	65	66	67
2	2	ECETOC TRA FLAT DATABASE			
760	760	Scaling output for Environment — Open Scaling output			
783	783				
784	784	Output for Scaling / DU ES Conformity Tool			
785	785	M_{SPERC} or M_{SITE} (kg/d)	9090.909091	300	WDU!
786	786	Receiving Water Dilution (Fresh or Marine)	10	10	-
787	787	Wastewater treatment plant flow (m^3/d)	2000	2000	-
788	788	Receiving water body flow rate (m^3/d) [for/alternative to dilution factor]			
789	789	Optional: Emission days per year	220	200	-
790	790	Onsite Removal Efficiency - Air (%)	0	80	-
791	791	Onsite Removal Efficiency - Wastewater (%)	75	90	-
792	792	Release rate air - after on-site RMMs (kg/day)	227.2727273	0.3	-
793	793	Release rate wastewater - after on-site RMMs (kg/day)	9.090909091	15	-
794	794	Municipal Sewage Treatment Plant (STP) used ?	yes	yes	-
795	795	Municipal Sewage Treatment Plant (STP) removal rate (%)	87.36698355	87.36698355	-
796	796	On-site (industrial) Sewage Treatment Plant used ?	yes		-
797	797	Municipal Sewage Sludge applied to soil?	no	no	-
798	798	Risk Driving Compartment (Code)	2	2	-
799	799	M_{SAFE} (kg/d)	15743.98289	315.569065	-
800	800	Risk Driving RCR - Air compartment driven	0.008396592	3.62253E-05	-
801	801	Risk Driving RCR - Water compartment driven	0.577421174	0.950663526	-

6. PRACTICAL CONSIDERATIONS FOR USERS

There are some known issues which need consideration when using the TRA integrated tool.

Microsoft Windows clipboard

Please be aware that the TRA, when calculating, uses a number of Microsoft Windows copy- paste functions. During this time values from different sheets are transferred to the Microsoft Windows clipboard. It is strongly advised to not using the windows clipboard during TRA calculation to avoid wrong information being put into the TRA from the Windows clipboard. This is extremely important when using the "run batch" mode.

CPU and RAM of your PC

The TRA uses as much CPU power as it can get. This means that during a large batch process it may happen that other work on the same computer may be very slow. However, if you have a multi-core CPU, the TRA uses only one core and other work on the same computer should not be affected too much.

It may also happen that the TRA requires a lot of memory (RAM) during operation (100 MB or more, depending on the number of entered data), especially when running a large batch process.

Country settings of your windows system

Please be aware that the country settings of your windows system may have an influence on the operation of the TRA. Lines 102/103 and 105/106 of the datasheets have a drop-down selection of "true" and "false", for example, for the approach you select for the environmental assessment (ERC, SpERC, release fractions, release rates). If your computer uses a different language than English, problems might occur because "true" and "false" are not the right words for your computer. If you cannot change your language and country settings to English, a workaround is to copy and paste the terms in your computers language into the fields rather than selecting them from the drop-down menu.

TIER II data

TIER II input data can be given for refining the assessments in lines 110-181 in the datasheets. Please consider that inputs made in these lines will only be taken into account when using the "run batch" mode in the user interface. Those data cannot be loaded into the user interface and will therefore not be considered in the "run" mode.

PNEC derivation

The PNEC derivation can also only be used in the "run batch" mode, not in the "run" mode.

Running "batch" mode for a single substance

Some functions like PNEC derivation or TIER II data are only taken into account by the tool, if "run batch" is selected in the user interface.

If you want to use these functions you need to calculate your substance(s) via the "run batch". The "run batch" can be used for many or for just one substance. Just specify the starting substance and the last

substance to be calculated in the user interface cells I26 and K26. If you want to run a "batch" for just one substance the start substance number (cell I26) and the end substance number (K26) are identical.

Differences between the consumers standalone version and the integrated version

For sentinel products, the stand-alone tool allows users to change product subcategory parameters within each sentinel group. This could result in changes in the worst-case scenario. In the Integrated Tool, users cannot change product subcategory parameters within each sentinel group so the worst-case scenario is always "fixed".