Targeted Risk Assessment

User Guide for the integrated tool
- Version 3.2

Brussels, October 2023

PREFACE

Changes in version 3.2 relate to the worker part of the tool (as documented in ECETOC TR 141). The consumer part of the tool has not been changed since version 3.1. In the environmental part of the tool, the built-in SpERC assessment via selection of industry sector, and subsequently the available SpERCs of the selected sector, was removed in version 3.2 because the SpERC input data were outdated and no full set of current SpERC data was available. SpERCs-based assessment can still be performed via the Datasheets using the TIER II environmental release estimation via release fractions (see details in Sections 3.7 and 5.2.2).

The changes to the TRA-Worker module are as follows:

- LEV efficiency for industrial PROC 7 (inhalation) has been reduced from 95% to 90%
- LEV efficiency for professional PROC 8b has been reduced from 90% to 80%
- Industrial PROC 10 medium volatility liquids base estimate has been increased from 50 ppm to 100 ppm (vapour).
- Professional PROC 10 medium volatility liquids base estimate has been increased from 100 ppm to 200 ppm (vapour).
- Industrial PROC 8a base estimate (liquids and solids) for dermal exposure increased from 13.71 to 27.43 mg/kg/day.
- Professional PROC 8a base estimate for dermal exposure (liquids and solids) increased from 13.71 to 27.43 mg/kg/day.

ECETOC's Targeted Risk Assessment (TRA) Tool can be found and downloaded here:

https://www.ecetoc.org/tools/tra-main/

ECETOC's Technical Reports (TR) including version releases and changes to the TRA Tool can be found here:

https://www.ecetoc.org/publications/technical-reports/

Table 1. Brief List of significant TRs for the TRA

Technical Reports	Version
140 and 141	3.2
124 and 131	3.1
114	3
107	2
93	1

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1. INTRODUCTION

This User Guide is to help the reader operate the ECETOC TRA v3.2 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 (TRs), a list of which can be found in Table 1, page 4, wherein detailed explanation of the basis for the TRA tool can be found. These TRs should help answer most technical questions concerning the tool.

Following the introduction of the 2007 REACH Regulation, the ECETOC TRA v2 was developed to account for exposure assessments needing to be reported for the development of Chemical Safety Assessments (CSAs) for relevant substances. V3 was launched in 2009. Subsequent to the first REACH registration deadline in 2010, v2 was further refined to account for the experiences gained during the first phase of REACH. V3 was launched in April 2012. The introduction of v3.1 of the TRA (launched June 2014) enabled the exposures and risks associated with the infrequent consumer uses of substances to be better addressed. Furthermore, the worker tool was updated in the current version 3.2 of the tool, following the publication of the ECETOC TRs 140 and TR 141 wherein a review of published studies on worker TRA tool performance were reviewed and consequently some updates to the worker TRA tool applied.

The ECETOC TRA integrated tool offers exposure and risk assessment for workers, consumers and the environment in one single tool, the so-called 'integrated' tool (named Targeted Risk Assessment Model 'TRAM' in the tool). In addition, the consumer and worker assessment tools are available as standalone versions, and have their own corresponding User Guides.

1.1 Manual and Batch Mode

The ECETOC TRA integrated tool can be operated in a manual and a batch mode. In the manual mode, assessments are performed and saved one-by-one. In essence, one substance can be assessed with up to fifteen scenarios in one single run. In contrast the batch mode allows for serial assessments and up to 60 scenarios per substance. Both modes are administered via the User Interface. In addition to the serial assessments, the batch mode allows for enhanced reporting of results and supports advanced environmental assessments.

1.2 Data Entry

Data entry can occur via the User Interface or via the Datasheets within the ECETOC TRA integrated tool. Assessments in batch mode require that data are entered into the Datasheets prior to the assessment. Alternatively, data entered in the User Interface may be stored to the Datasheets (see section 3.2).

1.3 Standard and Refined Assessments

Standard assessments can be performed in the manual and batch modes. Advanced assessments available in the manual mode include all refinements of worker assessments and generate customised subcategories for

consumer assessments. These options are also available via the batch mode which has an extended number of scenarios. The batch mode now exclusively allows the "manual SpERC" approach via the Datasheets using the TIER II environmental release estimation via release fractions (see details in Sections 3.7 and 5.2.2). In addition, the batch mode 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 REACH R16 Technical Guidance, and to generate customised emission assessments.

1.4   Working in EXCEL 2007 and 2010

The ECETOC TRA integrated tool has been developed in the 2003 version of EXCEL.

Different version of Excel (365 to 2003) differ in a small number of operations on account of altered structures and menu setups, however the assessment and results of the tool should stay consistent between excel versions.

Some of the menu changes will be addressed in Chapter 2.1 and 2.2 of this user guide.

2. STARTING / EXITING THE APPLICATION

2.1 Starting

To begin please follow the instructions on the ECETOC website (https://www.ecetoc.org/tools/tra-main/tra-download/) and download the Integrated tool.

Once downloaded, first extract the file "Integrated tool v3.2.zip" into one single folder using WinZip or any other program capable of extracting .zip-files.

After extracting the files the folder should look similarly to Figure 1.

Figure 1: Extracted ECETOC TRA integrated tool folder.

Before you run the application, right-click on the file "ecetocTRAM.xls" and go to properties. Under the General tab check the unblock security box at the bottom of the Properties window (Figure 2). This will unblock the macros for the tool.
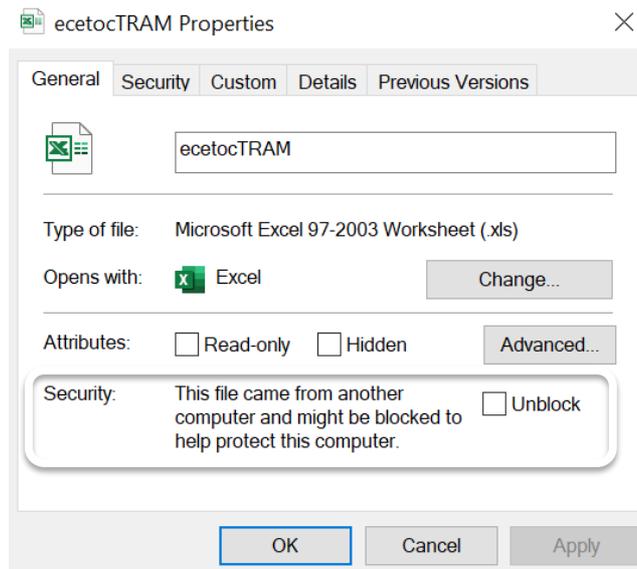
Figure 2: Unblock the TRA tool to enable Macros in Excel

Once this is done open "ecetocTRAM.xls" and the tool will start. If done correctly alongside the main Excel table eight other Excel instances should open (you may need to click on Enable content).

Troubleshooting: Enabling Macros inside Excel

Users of Excel 2007 and 2010 may have to enable the macros in the ECETOC TRA integrated tool as shown below.

If a security warning appears when you open "ecetocTRAM.xls" you can also enable macros when prompted in the security warning message box (Figure 3). This will also allow the remaining eight files to automatically open and link together.
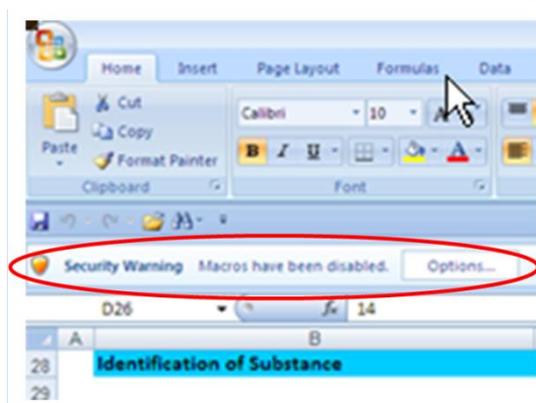
Figure 3: Security Warning prompt inside excel to enable macros

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 tab "Add-ins" in Excel (Figure 4 (a)) 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.

For excel versions 2007/2010, the "Save and exit" can also be accessed via "Add-ins" (Figure 4 (b)). For Excel 2003, this can be done via the ecetocTRAM button on the command line (Figure 4 (c)).

(a)
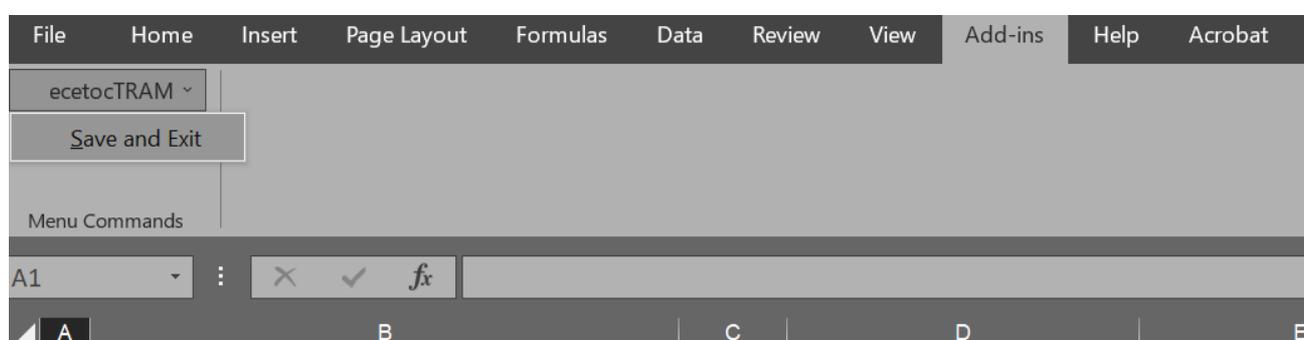
(b)
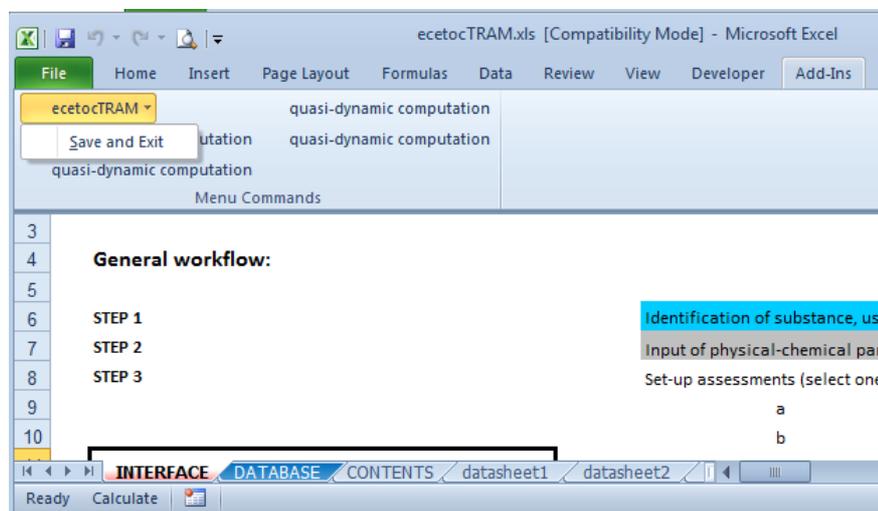
(c)
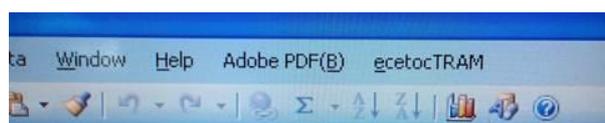
Figure 4: Examples for exiting the tool from the different excel versions (a) 365; (b) Excel 2007/2010; (c) Excel 2003

3. USER INTERFACE

3.1 Overview

The User Interface of the ECETOC TRA integrated tool 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-based exposure estimates. TIER II environmental estimates are possible via the Datasheets and using the batch mode exclusively, which includes assessments using the "manual SpERC" approach via the Datasheets using the TIER II environmental release estimation via release fractions (see details in Sections 3.7 and 5.2.2).

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.
  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 of the User Interface (Figure 5) 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 organisation or just speeds up the batch run if e.g., refinement of only one part is required.

New features included in versions 3.1 and 3.2 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 tool 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 TRA integrated tool 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 TRA integrated tool 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 "Save" function further down in this chapter).
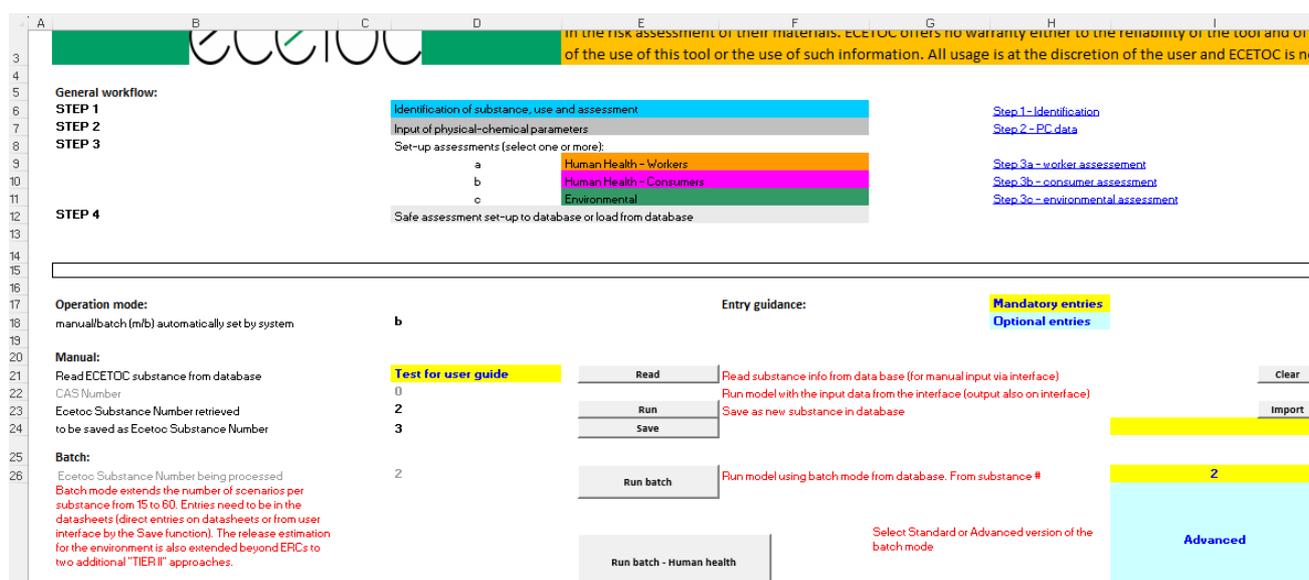
Figure 5: Overview of Part I of the User Interface

3.2.1 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 may be made).

3.2.2 Indicator: Manual or Batch Mode

Cell D18 indicates whether the tool is operating in manual ("m") or batch mode ("b"). This is not an entry field, but automatically set by the TRA integrated tool 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).

3.2.3 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 (Sections 3.3 – 3.7). The "Clear" button can be used to clear any existing entries in the User Interface in order to avoid confusion.

3.2.4 Run: Single Substance Assessment from User Interface in Manual Mode

To run the entered scenarios for the selected substance in the User Interface, simply click on the "Run" button in cell E22. 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).

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

To save a substance just entered into the "User 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 TRA integrated tool 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 TRA integrated tool 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.

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

In manual mode, a substance with its scenarios can be read 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 inputs for environmental assessments will be transferred (no TIER II assessments). ERC assessments will be assigned in rows 114-128 in the Interface.

3.2.7 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 "Save" function can be used to remove datasets from Datasheets to create a blank sheet for new entries.

3.2.8 Batch Mode

When processing data in the batch mode, it is necessary to enter the starting substance number into cell I26 of the interface 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 database and where.

By clicking "Run batch" in cell E26 of the interface, 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 of the interface).

3.2.9 Standard vs Advanced

Cell I27 in the User Interface allows the user to select a "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) (in Datasheets line 520 and below). It is also possible to derive PNEC by the model based on ecotoxicological data inputs in the Datasheets (refer to Section 5.2.4).

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 of the User Interface (Figure 6) asks the user to enter data for the identification of the substance to be assessed, like substance name and CAS number.

Figure 6: 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. 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 (Parts IV and V of the User Interface; Sections 3.5 and 3.6), because they directly determine the assessed scenarios.

3.4 Part III - General physico-chemical data entry

Part III of the User Interface (Figure 7) is the location 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 chemical class for Koc-QSAR. The fields displayed in blue are optional entries, but at least one of the optional fields needs to be filled in. Some fields (Partition coefficients octanol-water (K_{ow}) and organic carbon-water (K_{oc})) offer the selection of entering either the value for K_{ow} (cell D42) and K_{oc} (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 7: 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 and Chemical class for K_{oc} QSAR. Special fields are K_{ow}, K_{oc} and Vapour pressure: besides entering a value, the type of value needs to be selected from a drop-down menu (K_{ow} or log K_{ow}, K_{oc} or log K_{OC}, Pa or hPa). The fields displayed in blue are optional inputs, however one of the options must be used, either a chemical class for K_{oc}-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.

In cell G50 (Input for additional PC data) additional PC data (e.g. various solid-water partition coefficients, rate constants for various degradation reactions) can be entered, if a refinement for some reason 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 of the User Interface (Figure 8) 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 REACH 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). ECHA REACH Guidance R12v3 (2015) introduced PROC28 (maintenance activities) which is not included in the TRA.

Figure 8: 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. The use of LEV can be an effective means of reducing dermal exposure to chemicals. In a closed, continuous process with occasional controlled exposure the use of LEV can result in a reduction in dermal exposure of 90%. However, for processes where dermal exposure occurs due to direct contact with contaminated objects, or where the body/hands are positioned between the emission source and the LEV, use of LEV will hardly lead to a reduction of dermal exposure. Applying LEV reduction factors to the initial dermal exposure estimate is justifiable from a scientific point of view. However, the user should take a more conservative approach in using the LEV reduction factor for dermal exposure, when based on the description of working activities it is likely that the reduction of dermal exposure due to LEV is not very effective. For additional information on how LEV can affect dermal exposure the user is referred to ECETOC TR 114 (section 2.3).

Lines 76 to 79 represent entry fields for reference values (D76 or H76 and D77), 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/kg/day for (systemic) dermal exposure and µg/cm^2 for local dermal exposure). The type of value (e.g. DNEL, OEL, etc.) may be specified in the field "basis for reference value" (F76-F79). For more details on the single parameters please refer to the ECETOC Technical Reports (TR) 93 and 107 and 114.

Practical note: TRA integrated tool 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

3.6.1 Working with existing categories and sub-categories

Part V of the User Interface (Figure 9) 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). Each row represents one (contributing) consumer scenario. 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 REACH guidance R12.

Further down in the drop-down list, all other PCs and ACs are available for the creation of new subcategories (see below (section 3.6.2) for more information on new sub-categories).

In E83-E97 it is possible to 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 TRA consumer standalone tool user guidance.

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 Reports 93, 107 and the amendment to TR 107 (TR 124).

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/m3 or mg/kg/day).

Figure 9: Overview of the consumer input cells in the "Interface" sheet

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.

3.6.2 Creating New Sub-Categories

3.6.2.1 Working with new sub-categories

Columns D and E of the User Interface 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), intended to generate Specific Consumer Exposure Determinants (SCEDs) for common uses of consumer products, is referred to at this stage (and where SCED information can be found on the ENES website and the websites of CEFIC and various DUCC members).

Before new subcategories 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 9) and a macro will take the user to the 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 10). 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 sub-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.

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

Figures 10, 11, and 12 show the general, dermal and oral parts of the "Add Subcategories" sheet, respectively.

Column B in the sheet "Add Subcategories" 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 the user just needs to ensure to avoid duplications 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 (Figure 10)
- Routes of exposure and differentiation for adults and children in columns H-J (Figure 10)
- Product Ingredient Fraction by Weight in column K (Figure 10)
- Frequency of use – for all routes in column L (Figure 10)
- Dermal parameters in columns M and N (related contact area values returned in column O and P) (Figure 11)

- Oral parameters in columns Q, R and S (related contact area values returned in column T and U) (Figure 11)
- Inhalation parameters in columns V - Y (Figure 12)
- User comments can be captured in column AB (Figure 12)

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.

For more details on the use of new subcategories please refer to the updated user guide for the TRA consumer standalone tool (version 3.1).

Figure 10: General part of the input area for new sub-categories in the consumer sub-module, sheet "Add Subcategories"

Figure 11: Dermal and oral part of the input area for new sub-categories in the consumer sub-module, sheet "Add Subcategories"

Figure 12: Inhalation part of the input area for new sub-categories in the consumer sub-module, sheet "Add Subcategories"

Practical notes: When using "New sub-categories" created in the "Add-subcategories" sheet in the Consumer sub-module of the batch processing from 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 settings can only be changed in the "Add-subcategories" sheet.

3.7   Part VI - Data Entry for Environmental Assessment

Part VI of the User Interface (Figure 13) 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 REACH guidance R16.

The use of fully implemented Specific Environmental Release Categories (SpERCs) as in the original tool was de-activated in version 3.2 because the SpERC input data were outdated and no full set of current SpERC data was available. However, the TRA tool may still be used for assessment of such refined SpERC inputs via the Datasheets and the respective instructions are provided in Section 5.2.

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 (

Figure 13, Figure 14).

- The description of use (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 (E114-E128) needs to be entered as a number. In cells F114-F128 the fraction of the tonnage considered for a regional assessment is selected via a drop-down menu. Here a value of 1 (100%) or 0.1 (10%) can be selected in line with the ECHA guidance document R16. For more information on regional assessments please refer to the Technical Report 107 and the ECHA REACH guidance Part D and R16.
- In cells H114-H128, the ERC for the use has to be selected. A glossary for the ERCs can be found in line 131 and the ECHA REACH guidance document R16. Column I for these rows needs to be filled to specify if there is a sewage treatment plant considered for this scenario. Column G has been deactivated as SpERC assessments are no longer possible in v3.2 via the User Interface.

Further down (cells D135-D141) (Figure 15), 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 notes: 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 114.

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.

No.	Description of use	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)*	ERC (mandatory in all cases as use descriptor !)	for ERC approach STP for ERC (default is Yes, unless for ERC 1-7 and 12a, 12b direct discharge is given)
1		Manufacturing	1.00E+03	1	ERC1	yes
2		Formulation	1.00E+02	1	ERC2	yes
3		Formulation	1.00E+02	1	ERC2	no
4		Formulation	1.00E+02	1	ERC2	
5		Processing	1.00E+02	1	ERC4	yes
6		Processing	1.00E+02	0.1	ERC8a	yes
7		Processing	1.00E+02	0.1	ERC8c	yes
8						
9						
10						
11						
12						
13						
14						
15						

Environmental Assessment (including Man via Environment)

for debugging scenario no.   1

ERC glossary (text descriptions for reference): ERC10b Wide dispersive outdoor use of long-life articles and materials with high or intended release

Manual entry of reference values

		Basis of reference value
Microorganisms in STP	2.00E-01 mg L^{-1}	PNEC
Freshwater aquatic	3.00E-01 mg L^{-1}	PNEC
Freshwater sediment	4.00E-01 mg kg$_{dwt}$$^{-1}$	PNEC
Marine water	5.00E-01 mg L^{-1}	PNEC
Marine sediment	6.00E-01 mg kg$_{dwt}$$^{-1}$	PNEC
Terrestrial compartment	7.00E-01 mg kg$_{dwt}$$^{-1}$	PNEC
Secondary poisoning – for TIER II only	mg kg$_{feed}$$^{-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)	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.

* The most conservative assumption is that 100 % of the manufacturer's or importer's tonnage per year is applied at one site (i.e. fraction = 1). If it is known that the production or processing sites are numerous, various in size and randomly distributed over Europe, a "10 % rule" can be applied by assuming that 10 % of the amount produced or imported is used at the local scale (i.e. fraction = 0.1).

NOTE:

Defaults setting in TRA TIER I (ERC):
No STP marine and no primary settler are set per default in ERC assessments. STP settings can be adjusted in batch mode in the DATASHEETs.

PNEC secondary poisoning, PNEC freshwater-intermittent, and PNECmarine.water.intermittent addressed in TIER II (advanced batch mode) batch mode only

Input of (eco)toxicological data for PNEC derivation can be done in row 188 of datasheets. The model needs to be run in batch mode – Advanced to activate this functionality.

Figure 13: Part VI. Environmental exposure assessment input

	D	E	F	G	H	I
112						for ERC approach
113	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)*		ERC (mandatory in all cases as use descriptor !)	STP for ERC (default is Yes, unless for ERC 1-7 and 12a, 12b direct discharge is given)
114	Manufacturing	1.00E+03	1		ERC1	yes
115	Formulation	1.00E+02	1		ERC2	yes
116	Formulation	1.00E+02	1		ERC2	yes
117	Formulation	1.00E+02	1		ERC2	yes
118	Processing	1.00E+02	1		ERC4	yes
119	Processing	1.00E+02	0.1		ERC8a	yes
120	Processing	1.00E+02	0.1		ERC8c	yes
121						
122						
123						
124						
125						
126						
127						
128						

Figure 14: Part VI. Environmental exposure assessment input – General and ERC input

	A	B	C	D	E	F
133						
134		Manual entry of reference values				Basis of reference value
135		Microorganisms in STP		2,00E-01	mg L^{-1}	PNEC
136		Freshwater aquatic		3,00E-01	mg L^{-1}	PNEC
137		Freshwater sediment		4,00E-01	mg kg$_{dwt}$$^{-1}$	PNEC
138		Marine water		5,00E-01	mg L^{-1}	PNEC
139		Marine sediment		6,00E-01	mg kg$_{dwt}$$^{-1}$	PNEC
140		Terrestrial compartment		7,00E-01	mg kg$_{dwt}$$^{-1}$	PNEC
141		Secondary poisoning - for TIER II only			mg kg$_{food}$$^{-1}$	PNEC
142		Freshwater aquatic, intermittent release - for TIER II only			mg L^{-1}	PNEC
143		Marine water, intermittent release - for TIER II only			mg L^{-1}	PNEC
144		Man via the environment (total daily intake)		4,80E+01	mg kg$_{bw}$$^{-1}$ d^{-1}	DNEL
145		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.				

Figure 15: Part VI. Environmental exposure assessment input – Reference value input

4. OUTPUT OF RESULTS IN THE USER INTERFACE

The outputs (exposure estimates and risk characterisation ratios) 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).

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 (DENL, PNEC etc). If an RCR ≥1 is estimated for a use, the respective cell is highlighted in red.

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 (Figure 16). 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) are included in the assessment. If for a certain route (inhalative or dermal) no exposure can be estimated the result is #NV. Columns V to Z show the RCRs for the corresponding routes.

Figure 16: 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 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 T. Particularly the assumed effectiveness of LEV for inhalation exposure (and dermal exposure, where applicable) is reported. The assumed effectiveness is based on a value that might reasonably be anticipated for the workgroup (PROC) if a LEV system is properly designed, installed, operated and maintained. As such, this value can differ significantly from the actual effectiveness in any workplace.

4.2 Output of the Consumer Exposure and Risk

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/sentinel products. Red fields indicate an RCR>1, green fields indicate an RCR≤1.

The consumer results are structured in the same way as the worker results with one exception: Columns N-V show the results calculated for the product subcategories (if a product or article subcategory was specified)

(Figure 17) and columns X-AF show the results calculated for the "sentinel" product categories (if no product or article sub-category was specified) (Figure 18). For details on subcategories and sentinel products please refer to the TRA user guide for the standalone consumer tool.

Practical notes: Empty lines may occur if no sub-category was specified and, thus, only results for sentinel products were calculated (see Figure 18).

No sentinel product results will be reported for NEW sub-categories created by the user (see example in row 10 in Figure 18).

	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
81 OUTPUT BY PRODUCT SUBCATEGORY									
83	1.34E-03	1.19E-01		1.47E-02		2.94E-03	1.19E-01		1.22E-01
84	2.14E-03	2.14E+01		1.56E-02		3.12E-03	2.14E+01		2.14E+01
85	5.38E-01	2.38E+00		5.88E+00		1.18E+00	2.38E+00		3.56E+00
86	1.43E-03	1.43E+01		1.56E-02		3.12E-03	1.43E+01		1.43E+01
87									
88	3.15E+00	2.38E-01		1.72E+01		3.45E+00	2.38E-01		3.69E+00
89	7.84E-04	1.43E+01		1.56E-02		3.12E-03	1.43E+01		1.43E+01
90	1.08E+02	7.15E+00		2.16E+03		4.31E+02	7.15E+00		4.38E+02
91									
92									
93									
94									
95									
96									
97									

Figure 17: Consumer output fields for Product Subcategory in the User Interface

Footnote: Red fields indicate an RCR>1, green fields indicate an RCR≤1

	X	Y	Z	AA	AB	AC	AD	AE	AF
81	OUTPUT BY SENTINEL PRODUCT CATEGORY								
82	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 Exposure
83	1.03E+02	4.29E+01	0.00E+00	1.13E+03		2.25E+02	4.29E+01	0.00E+00	2.68E+02
84	1.03E+02	2.14E+01	0.00E+00	1.13E+03		2.25E+02	2.14E+01	0.00E+00	2.46E+02
85	2.14E-03	4.29E+01	0.00E+00	1.56E-02		3.12E-03	4.29E+01	0.00E+00	4.29E+01
86	1.03E+02	4.29E+01	0.00E+00	1.13E+03		2.25E+02	4.29E+01	0.00E+00	2.68E+02
87	4.97E+00	5.95E-02	0.00E+00	8.70E+02		1.74E+02	5.95E-02	0.00E+00	1.74E+02
88	4.97E+00	2.38E-01	0.00E+00	8.70E+02		1.74E+02	2.38E-01	0.00E+00	1.74E+02
89	4.72E+01	1.29E+02	0.00E+00	6.26E+03		1.25E+03	1.29E+02	0.00E+00	1.38E+03
90	4.72E+01	1.29E+02	0.00E+00	6.26E+03		1.25E+03	1.29E+02	0.00E+00	1.38E+03
91	4.72E+01	1.29E+02	0.00E+00	6.26E+03		1.25E+03	1.29E+02	0.00E+00	1.38E+03
92	1.03E+02	4.29E+01	0.00E+00	1.13E+03		2.25E+02	4.29E+01	0.00E+00	2.68E+02
93	#N/A	#N/A	#N/A	#N/A		#N/A	#N/A	#N/A	#N/A
94	#N/A	#N/A	#N/A	#N/A		#N/A	#N/A	#N/A	#N/A
95	#N/A	#N/A	#N/A	#N/A		#N/A	#N/A	#N/A	#N/A
96	#N/A	#N/A	#N/A	#N/A		#N/A	#N/A	#N/A	#N/A
97	#N/A	#N/A	#N/A	#N/A		#N/A	#N/A	#N/A	#N/A

Figure 18: Consumer output fields for Sentinel Products in the User Interface

Footnote: Red fields (none in this example) indicate an RCR>1, green fields indicate an RCR≤1

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

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 (Figure 19). Red fields indicate an RCR>1, green fields indicate an RCR≤1.

The environment results are structured in the same way as the results for workers and consumers. 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 19). For details on this parameter please refer to Technical Reports 107 and 114.

Figure 19: Environmental output fields in the User Interface

Footnote: Red fields indicate an RCR>1, green fields indicate an RCR≤1

All uses assessed separately:

	PEC in STP (mg.L⁻¹)	PEC for local freshwater (mg.L⁻¹)	PEC for local freshwater sediment (mg.kg_dwt⁻¹)	PEC for local soil (mg.kg_dwt⁻¹)	PEC for local marine water (mg.L⁻¹)	PEC for local marine sediments (mg.kg_dwt⁻¹)	Total daily intake man via the environment regional (mg.kg_bw⁻¹.d⁻¹)	RCR in STP	RCR for local freshwater	RCR for local freshwater sediment	RCR for local terrestrial environment	RCR for local marine water	RCR for local marine sediments	RCR for humans via the environment regional
114	1.48E+03	1.48E+02	2.01E+03	3.05E+02	1.48E+01	2.01E+02	1.15E-03	7.41E+03	4.94E+02	5.04E+03	4.36E+02	2.96E+01	3.36E+02	2.31E-03
115	9.88E+01	9.88E+00	1.34E+02	2.03E+01	9.88E-01	1.34E+01	1.15E-03	4.94E+02	3.29E+01	3.36E+02	2.90E+01	1.98E+00	2.24E+01	2.31E-03
116	9.88E+01	9.88E+00	1.34E+02	2.03E+01	9.88E-01	1.34E+01	1.15E-03	4.94E+02	3.29E+01	3.36E+02	2.90E+01	1.98E+00	2.24E+01	2.31E-03
117	9.88E+01	9.88E+00	1.34E+02	2.03E+01	9.88E-01	1.34E+01	1.15E-03	4.94E+02	3.29E+01	3.36E+02	2.90E+01	1.98E+00	2.24E+01	2.31E-03
118	2.47E+03	2.47E+02	3.36E+03	5.10E+02	2.47E+01	3.36E+02	1.15E-03	1.23E+04	8.23E+02	8.39E+03	7.28E+02	4.94E+01	5.60E+02	2.31E-03
119	2.71E-02	1.12E-02	1.52E-01	2.91E-02	1.13E-03	1.53E-02	1.15E-03	1.35E-01	3.73E-02	3.80E-01	4.15E-02	2.25E-03	2.55E-02	2.31E-03
120	2.71E-04	8.50E-03	1.16E-01	2.36E-02	8.58E-04	1.17E-02	1.15E-03	1.35E-03	2.83E-02	2.89E-01	3.38E-02	1.72E-03	1.94E-02	2.31E-03
123	2.73E-02	1.12E-02	4.65E-02	2.63E-02	1.13E-03	4.60E-03		1.37E-01	3.74E-02	1.16E-01	3.76E-02	2.26E-03	7.66E-03	

	Msafe in STP (kg.day⁻¹)	Msafe freshwater (kg.day⁻¹)	Msafe freshwater sediments (kg.day⁻¹)	Msafe terrestrial (kg.day⁻¹)	Msafe marine water (kg.day⁻¹)	Msafe marine sediments (kg.day⁻¹)	Msafe humans (kg.day⁻¹)		STP used?	Removal in STP	Source of information on RMM and related effectiveness considered in spERC	Release to waste (for information only) [%]
114	6.75E+00	1.01E+02	9.93E+00	1.15E+02	1.69E+03	1.49E+02	2.17E+07		yes	0.0123		
115	2.03E+01	3.04E+02	2.98E+01	3.45E+02	5.06E+03	4.46E+02	4.33E+06		yes	0.0123		
116	2.03E+01	3.04E+02	2.98E+01	3.45E+02	5.06E+03	4.46E+02	4.33E+06		yes	0.0123		
117	2.03E+01	3.04E+02	2.98E+01	3.45E+02	5.06E+03	4.46E+02	4.33E+06		yes	0.0123		
118	4.05E-01	6.08E+00	5.96E-01	6.87E+00	1.01E+02	8.93E+00	2.17E+06		yes	0.0123		
119	4.05E-01	1.47E+00	1.44E-01	1.32E+00	2.43E+01	2.15E+00	2.37E+01		yes	0.0123		
120	4.05E+01	1.93E+00	1.90E-01	1.62E+00	3.19E+01	2.82E+00	2.37E+01		yes	0.0123		

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 to the Datasheets via the save button in the User Interface (limited to 15 uses) or by direct entry into the Datasheets (see Section 3.2 for more information on data entry). Entering data directly into the Datasheets is only recommended for advanced users. Doing it this way offers the possibility of entering new data necessary for further refinements. 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 20). 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. Yellow fields are mandatory inputs, blue fields are optional, as in the User Interface. 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 (Figure 20)).

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 (more information in Section 3.2). 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 20: Upper part of a Datasheet, including the worker input part

Footnote: One use is represented in one column (red box).

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 User Interface sheet are available, but in columns instead of rows (same as for worker assessments) (Figure 21). The button to navigate to the consumer sub-module to create or edit new sub-categories is located in column B (cell B53).

Figure 21: Consumer input part of a Datasheet

Footnote: One use is represented in one column (red box).

5.2 Datasheets – Data Input for Advanced Assessments

5.2.1 Environmental Emission Assessment via Datasheet

All entries for refinement are formatted as "optional" (blue fields; i.e. not required), but are required for TIER II environmental exposure assessments.

The assessment via pre-populated SpERC data was deactivated in v3.2 of the tool. The new approach for SpERC-based assessments is addressed in Section 5.2.2

The selection of the release estimation method/approach for environmental assessments in the Datasheets is done via three drop-down cells (lines 102 (ERC-based), 105 (SpERC-based) and 106 (based on measured data) - see Figure 22). Only one can be set to "TRUE" (warning message will appear in line 107 if more than 1 "TRUE" was selected).

	A	B	D
1	1	2	4
2	2	**ECETOC TRA FLAT DATABASE**	
3	3		1
102	102	Select approach ERC	TRUE
103			
104	104	TIER II Assessment Approaches:	
105	105	Select approach using SPECIFIC RELEASE FRACTIONS	TRUE
106	106	Select appraoch using MEASURED DATA (releases in kg/day)	FALSE
107	107	**ECETOC TRA FLAT DATABASE - INPUT TIER 2**	only 1 TRUE

Figure 22: Selection of the release estimation method for environmental assessments in the Datasheets

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

5.2.2 "Manual SpERC" Assessments and Refining Environmental Assessments beyond SpERCs

Lines 109-181 are for entering input parameters for a refined environmental assessment including SpERC assessments   (

	A	B	D
1	1	2	4
2	2	**ECETOC TRA FLAT DATABASE**	
3	3		1
102	102	Select approach ERC	FALSE
103			
104	104	TIER II Assessment Approaches:	
105	105	Select approach using SPECIFIC RELEASE FRACTIONS	TRUE
106	106	Select appraoch using MEASURED DATA (releases in kg/day)	FALSE
107	107	**ECETOC TRA FLAT DATABASE - INPUT TIER 2**	
108	108	**Environmental Assessment (including Man via Environment)**	
109	109	**Justifications for refined release parameters**	
110	110	Basis used for refinement (e.g. ERC, SPERC)	
111	111	Fraction of EU tonnage to region (-) - modified in line 78	
112	112	Daily amount used at site [kg/d]	
113	113	Release times per year (d/year)	
114	114	Local release to air - RMM	
115	115	Local release to air - efficiency of RMM (%)	
116	116	Local release to sewage - RMM (beyond municipal STP)	
117	117	Local release to sewage - efficiency of RMM (%) [default for on-site STP is same as municipal STP]	
118	118	Local release to soil - RMM	
119	119	Local release to soil - efficiency of RMM (%)	
120	120	**RELEASE ESTIMATION BASED ON SPECIFIC RELEASE FRACTIONS**	
121	121	Comments 1	
122	122	Comments 2	
123	123	Daily amount used at site [kg/d] (release fractions)	
124	124	Release times per year (d/year)	
125	125	Local release fraction to air	
126	126	Local release fraction to sewage	
127	127	Local release fraction to soil	
128	128		
129	129	**RELEASE ESTIMATION BASED ON RELEASE RATES, e.g. measured data (releases in kg/day)**	
130	130	Daily amount used at site [kg/d] (release rates)	
131	131	Release times per year (d/year)	
132	132	Name of Monitoring Site or other source of information	
133	133	Remark	
134	134	Monitoring regime	
135	135	Remark	
136	136	Measured. Release to air (kg/d)	

Figure 23). 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 SpERC documents or OECD emission scenario documents), 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 notes: TRA integrated tool 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- or 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:

$$Refined\ release\ fraction = Original\ release\ fraction \cdot (1 - Efficiency\ of\ RMM)$$

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

$$Refined\ release\ fraction = 0.02 \cdot (1 - D115)$$

	A	B	D
1	1	2	4
2	2	**ECETOC TRA FLAT DATABASE**	
3	3		1
102	102	Select approach ERC	FALSE
103	103		
104	104	TIER II Assessment Approaches:	
105	105	Select approach using SPECIFIC RELEASE FRACTIONS	TRUE
106	106	Select approach using MEASURED DATA (releases in kg/day)	FALSE
107	107	**ECETOC TRA FLAT DATABASE - INPUT TIER 2**	
108	108	**Environmental Assessment (including Man via Environment)**	
109	109	**Justifications for refined release parameters**	
110	110	Basis used for refinement (e.g. ERC, SPERC)	
111	111	Fraction of EU tonnage to region (-) - modified in line 78	
112	112	Daily amount used at site [kg/d]	
113	113	Release times per year (d/year)	
114	114	Local release to air - RMM	
115	115	Local release to air - efficiency of RMM (%)	
116	116	Local release to sewage - RMM (beyond municipal STP)	
117	117	Local release to sewage - efficiency of RMM (%) [default for on-site STP is same as municipal STP]	
118	118	Local release to soil - RMM	
119	119	Local release to soil - efficiency of RMM (%)	
120	120	**RELEASE ESTIMATION BASED ON SPECIFIC RELEASE FRACTIONS**	
121	121	Comments 1	
122	122	Comments 2	
123	123	Daily amount used at site [kg/d] (release fractions)	
124	124	Release times per year (d/year)	
125	125	Local release fraction to air	
126	126	Local release fraction to sewage	
127	127	Local release fraction to soil	
128	128		
129	129	**RELEASE ESTIMATION BASED ON RELEASE RATES, e.g. measured data (releases in kg/day)**	
130	130	Daily amount used at site [kg/d] (release rates)	
131	131	Release times per year (d/year)	
132	132	Name of Monitoring Site or other source of information	
133	133	Remark	
134	134	Monitoring regime	
135	135	Remark	
136	136	Measured. Release to air (kg/d)	

Figure 23: Optional input for a TIER II environment assessment with release estimates based on release fraction, e.g. from SpERC documents or OECD emission scenario documents or release rates, e.g. from measured data

5.2.3 Refined Physical-Chemical and Degradation Data

Some additional physical-chemical data and degradation rates can be entered for a refined environmental assessment (Figure 24).

	A	B	D
1	1	2	4
2	2	**ECETOC TRA FLAT DATABASE**	
3	3		1
163	163		
164	164	**PHYSICAL-CHEMICAL SUBSTANCE PROPERTIES**	
165	165	Vapour pressure at the temperature of the data set (Pa) - from TIER I	
166	166	Temperature at which vapour pressure was measured (degrees C)	25
167	167	Water solubility at the temperature of the data set (mg.l-1) - from TIER I	
168	168	Temperature at which solubility was measured (degrees C)	
169	169	Melting point (degrees C)	
170	170	Solids-water partition coefficient raw sewage sludge (l.kg-1)	
171	171	Solids-water partition coefficient settled sewage sludge (l.kg-1)	
172	172	Solids-water partition coefficient activated sewage sludge (l.kg-1)	
173	173	Solids-water partition coefficient effluent sewage sludge (l.kg-1)	
174	174		
175	175	*DEGRADATION AND TRANSFORMATION RATES*	
176	176	Rate constant for degradation in STP (d-1)	
177	177	Total rate constant for degradation in surface water at env. Temp (d-1)	
178	178	Total rate constant for degradation in marine water at env. Temp (d-1)	
179	179	Total rate constant for degradation in bulk sediment at env. Temp (d-1)	
180	180	Rate constant for degradation in air (d-1)	
181	181	Total rate constant for degradation in bulk soil at env. Temp (d-1)	0.005

Figure 24: Optional input of refined physical-chemical and degradation data for a TIER II environment assessment

5.2.4 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 (

	A	B	C
1	1	2	3
2	2	**ECETOC TRA FLAT DATABASE**	1
3	3		0
182	182		
183	183	Environmental Assessment - PNEC derivation	
184	184		
185	185	*TOXICOLOGICAL SUBSTANCE PROPERTIES*	
186	186	**Toxicity to micro-organisms (mg.l-1)**	
187	187	*Respiration inhibition EU Annex V C.11, OECD 209*	
188	188	EC50 for micro-organisms in an STP	
189	189	EC10 for micro-organisms in an STP	
190	190	NOEC for micro-organisms in an STP	
191	191	*Inhibition control in base set tests*	
192	192	NOEC for micro-organisms in an STP	
193	193	*Activitated sludge growth inhibition, ISO-15522*	
194	194	EC50 for micro-organisms in an STP	
195	195	EC10 for micro-organisms in an STP	
196	196	NOEC for micro-organisms in an STP	
197	197	*Pilot scale activated sludge simulation tests, OECD 303 A, ISO-11733*	
198	198	NOEC for micro-organisms in an STP	
199	199	*Inhibition of nitrification, ISO-9509*	
200	200	EC50 for micro-organisms in an STP	
201	201	EC10 for micro-organisms in an STP	
202	202	NOEC for micro-organisms in an STP	
203	203	*Ciliate growth inhibition tests,*	
204	204	EC50 for micro-organisms in an STP	
205	205	EC10 for micro-organisms in an STP	
206	206	NOEC for micro-organisms in an STP	
207	207	*Growth inhibition tests with Pseudomonas putida, NF EN ISO 10712*	
208	208	EC50 for micro-organisms in an STP	
209	209	EC10 for micro-organisms in an STP	
210	210	NOEC for micro-organisms in an STP	
211	211	**Aquatic toxicity**	
212	212	*Fresh water (mg.l-1)*	
213	213	LC50 for fish	
214	214	L(E)C50 for crustaceans	
215	215	EC50 for algae	
216	216	LC50 for additional taxonomic group	
217	217	NOEC for fish	
218	218	NOEC for crustaceans	
219	219	NOEC for algae	
220	220	NOEC for additional taxonomic group 1	
221	221	NOEC for additional taxonomic group 2	
222	222	NOEC for additional taxonomic group 3	
223	223	NOEC for additional taxonomic group 4	

Within row 183: *Open PNEC derivation area* / *Hide PNEC derivation area*

Figure 25). This option is only available in the "advanced" batch mode.

However, many users will have derived PNECs outside of the TRA integrated tool and will not use these rows. Therefore, a feature is included 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 25: Optional input for PNEC derivation based on (eco)toxicological data

Practical note: 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 Datasheets - Output

The output within the Datasheets is structured in the same way as the input: worker (see example in Figure 26), consumer, environment (example in Figure 27). Environment TIER II output follows. 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 arranged 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).

		C	D	E	F	G	H
1	2	3	4	5	6	7	8
2	ECETOC TRA FLAT DATABASE	1					
3		0	1	2	3	4	5
444	ECTETOC TRA FLAT DATABASE - OUTPUT TIER 1						
445							
446	Human Health - Workers						
447	Estimate of exposures						
448	Long-term Inhalative Exposure Estimate (ppm volatiles/mg.m-3 solids)		0.01	0.02	0.7	0.018	0.0042
449	Long-term Inhalative Exposure Estimate (mg/m3)		0.322083333	0.644166667	0.7	0.57975	0.135275
450	Long-term Dermal Exposure Estimate (mg/kg/day)		0.034285714	0.274285714	0.068571429	6.857142857	0.041142857
451	Short-term Inhalation Exposure Estimate (mg/m3)		0.322083333	0.644166667	2.8	0.96625	0.135275
452	Long-term Local Dermal Exposure Estimate (µg/cm2)		10	40	20	1000	6
453	Notes/comments on exposure estimates:			LEV efficiency inhalation [%]: 80, LEV efficiency demal [%]: 0,			LEV efficiency inhalation [%]: 90, LEV efficiency demal [%]: 90,
454	Risk characterization						
455	Risk Characterisation Ratio - Long-term Inhalation		0.032208333	0.064416667	0.07	0.057975	0.0135275
456	Risk Characterisation Ratio - Long-term Dermal		0.006857143	0.054857143	0.013714286	1.371428571	0.008228571
457	Risk Characterisation Ratio - Long-term Total Exposure		0.039065476	0.11927381	0.083714286	1.429403571	0.021756071
458	Risk characterisation Ratio - Short-term Inhalation		0.016104167	0.032208333	0.14	0.0483125	0.00676375
459	Risk characterisation Ratio - Long-term Local Dermal		No Local Dermal DNEL	No Local Dermal DNEL	No Local Dermal DNEL	No Local Dermal DNEL	No Local Dermal DNEL

Figure 26: Output of a worker assessment within the Datasheets

		D	E
1	2	4	5
2	**ECETOC TRA FLAT DATABASE**		
3		1	2
488	**Environmental Assessment (including Man via Environment)**		
489	----- Plausibility check for regional tonnage ----		
490	**PEC**		
491	PEC in STP (mg.l-1)	0.027058945	0.000270589
492	PEC for local freshwater (mg.l-1)	0.011182491	0.008504057
493	PEC for local freshwater sediment (mg.kg$_{dwt}$-1)	0.152081877	0.115655178
494	PEC for local soil (mg.kg$_{dwt}$-1)	0.029070542	0.023631178
495	PEC for local marine water (mg.l-1)	0.001125808	0.000857964
496	PEC for local marine sediment (mg.kg$_{dwt}$-1)	0.015310987	0.011668317
497	Total daily intake man via the environment regional (mg.kgdw-1.d-1)	0.001154356	0.001154356
498			
499	**RCR**		
500	RCR in STP (-)	0.135294723	0.001352947
501	RCR for local freshwater (-)	0.03727497	0.028346857
502	RCR for local freshwater sediment (-)	0.380204693	0.289137946
503	RCR for local terrestrial environment (-)	0.041529346	0.033758825
504	RCR for local marine water (-)	0.002251616	0.001715929
505	RCR for local marine sediments (-)	0.025518311	0.019447195
506	RCR for humans via the environment (-)	0.002308481	0.002308481
507			
508	**Msafe**		
509	Msafe in STP (kg.d-1)	0.405001167	40.50011667
510	Msafe freshwater (kg.d-1)	1.470008445	1.933001592
511	Msafe freshwater sediments (kg.d-1)	0.144118475	0.18950996
512	Msafe terrestrial (kg.d-1)	1.31941688	1.623116933
513	Msafe marine water (kg.d-1)	24.3356448.9	31.93286058
514	Msafe marine sediments (kg.d-1)	2.147262784	2.817605345
515	Msafe human via the environment (kg.d-1)	23.73617584	23.73617584
516	Municipal STP used?	yes	yes
517	Removal in STP (fraction)	0.0123	0.0123

Figure 27: Output of an environmental assessment within the Datasheets providing the PECs, RCRs and M$_{safe}$ values per compartment

5.3.1 Interim Results of the Environmental Emission Assessment

Lines 151-162 display the results of the emission assessment (see

	A	B	C	D	E
1	1	2	3	4	5
2	2	**ECETOC TRA FLAT DATABASE**	1		
3	3		0	1	2
148	148	**VOLUMES and RELEASES (INTERIM RESULTS)**			
149	149	EU tonnage for use (tpa)			
151	151	Amount used locally (kg/d)		5.00E+04	1.00E+04
152	152	Release times per year (d/year)		2.00E+01	1.00E+01
153	153	Release fraction air (as in ERC or SPERC background table or set in line 125)		5.00E-02	2.50E-02
154	154	Release fraction (waste) water (as in ERC or SPERC background table or set in line 126)		6.00E-02	2.00E-02
155	155	Release fraction soil (as in ERC or SPERC background table or set in line 127)		1.00E-04	1.00E-04
156	156	Local release to air (kg/d) (will be set to 0 for WDU - see ECHA guidance R.16)		2.50E+03	2.50E+02
157	157	Local release to waste water (kg/d)		3.00E+03	2.00E+02
158	158	Local release to soil (kg/d) (will be set to 0 for WDU - see ECHA guidance R.16)		5.00E+00	1.00E+00
159	159	Regional release (from all uses) to air (kg/d)	463.0136986		
160	160	Regional release (from all uses) to waste water (kg/d)	385.9726027		
161	161	Regional release (from all uses) to fresh water directly (kg/d)	95.52821918		
162	162	Regional release (from all uses) to soil (kg/d)	14.05479452		

Figure 28). 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.

	A	B	C	D	E
1	1	2	3	4	5
2	2	**ECETOC TRA FLAT DATABASE**	1		
3	3		0	1	2
148	148	**VOLUMES and RELEASES (INTERIM RESULTS)**			
149	149	EU tonnage for use (tpa)			
151	151	Amount used locally (kg/d)		5.00E+04	1.00E+04
152	152	Release times per year (d/year)		2.00E+01	1.00E+01
153	153	Release fraction air (as in ERC or SPERC background table or set in line 125)		5.00E-02	2.50E-02
154	154	Release fraction (waste) water (as in ERC or SPERC background table or set in line 126)		6.00E-02	2.00E-02
155	155	Release fraction soil (as in ERC or SPERC background table or set in line 127)		1.00E-04	1.00E-04
156	156	Local release to air (kg/d) (will be set to 0 for WDU - see ECHA guidance R.16)		2.50E+03	2.50E+02
157	157	Local release to waste water (kg/d)		3.00E+03	2.00E+02
158	158	Local release to soil (kg/d) (will be set to 0 for WDU - see ECHA guidance R.16)		5.00E+00	1.00E+00
159	159	Regional release (from all uses) to air (kg/d)	463.0136986		
160	160	Regional release (from all uses) to waste water (kg/d)	385.9726027		
161	161	Regional release (from all uses) to fresh water directly (kg/d)	95.52821918		
162	162	Regional release (from all uses) to soil (kg/d)	14.05479452		

Figure 28: Example output of Interim results for volumes and releases in environment assessments

In the versions 3.1 and 3.2 of the TRA integrated tool additional output for the environmental assessments can be found at the bottom of the Datasheets (Figure 29), that correspond to REACH Chemical Safety Report Template (ECHA ES format).

1	2	4	5	6	7	8	9	10
2	ECETOC TRA FLAT DATABASE							
3		1	2	3	4	5	6	7
802								
803	NEW ECHA CSR Template							
804	Local concentrations for MvE - oral route							
805	Drinking water	1.35E+02	9.00E+00	9.00E+00	9.00E+00	2.26E+02	1.35E-02	1.11E-02
806	Fish	1.15E+01	3.93E-01	3.93E-01	3.93E-01	1.91E+01	1.58E-02	1.20E-02
807	Leaf crops	5.53E+02	3.55E+01	3.55E+01	3.55E+01	9.50E+02	4.85E-02	4.01E-02
808	Root crops	1.28E+02	8.48E+00	8.48E+00	8.48E+00	2.13E+02	1.27E-02	1.04E-02
809	Meat	1.62E-02	1.01E-03	1.01E-03	1.01E-03	2.87E-02	2.85E-06	2.64E-06
810	Milk	1.62E-01	1.01E-02	1.01E-02	1.01E-02	2.87E-01	2.85E-05	2.64E-05
811								
812	Regional concentrations for MvE - oral route							
813	Drinking water	1.19E-02	1.19E-02	1.19E-02	1.19E-02	1.19E-02	1.19E-02	1.19E-02
814	Fish	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02
815	Leaf crops	4.28E-02	4.28E-02	4.28E-02	4.28E-02	4.28E-02	4.28E-02	4.28E-02
816	Root crops	1.12E-02	1.12E-02	1.12E-02	1.12E-02	1.12E-02	1.12E-02	1.12E-02
817	Meat	2.82E-06	2.82E-06	2.82E-06	2.82E-06	2.82E-06	2.82E-06	2.82E-06
818	Milk	2.82E-05	2.82E-05	2.82E-05	2.82E-05	2.82E-05	2.82E-05	2.82E-05
819								
820	Local contribution to oral route (dose)							
821	Drinking water	3.87E+00	2.57E-01	2.57E-01	2.57E-01	6.46E+00	3.85E-04	3.16E-04
822	Fish	1.88E-02	6.46E-04	6.46E-04	6.46E-04	3.14E-02	2.59E-05	1.97E-05
823	Leaf crops	9.48E+00	6.08E-01	6.08E-01	6.08E-01	1.63E+01	8.31E-04	6.87E-04
824	Root crops	7.00E-01	4.65E-02	4.65E-02	4.65E-02	1.17E+00	6.98E-05	5.73E-05
825	Meat	6.99E-05	4.33E-06	4.33E-06	4.33E-06	1.23E-04	1.22E-08	1.13E-08
826	Milk	1.30E-03	8.07E-05	8.07E-05	8.07E-05	2.30E-03	2.28E-07	2.11E-07
827								
828	Regional contribution to oral route (dose)							
829	Drinking water	3.39E-04	3.39E-04	3.39E-04	3.39E-04	3.39E-04	3.39E-04	3.39E-04
830	Fish	1.96E-05	1.96E-05	1.96E-05	1.96E-05	1.96E-05	1.96E-05	1.96E-05
831	Leaf crops	7.34E-04	7.34E-04	7.34E-04	7.34E-04	7.34E-04	7.34E-04	7.34E-04
832	Root crops	6.14E-05	6.14E-05	6.14E-05	6.14E-05	6.14E-05	6.14E-05	6.14E-05
833	Meat	1.21E-08	1.21E-08	1.21E-08	1.21E-08	1.21E-08	1.21E-08	1.21E-08
834	Milk	2.26E-07	2.26E-07	2.26E-07	2.26E-07	2.26E-07	2.26E-07	2.26E-07

Figure 29: Example output of additional assessment results for the environmental compartment for the REACH Chemical Safety Report template

5.3.2 Scaling Parameters for Environmental Scenarios Assessed

A specific output section is included in the TRA integrated tool v3 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 lines 760 and below of the Datasheets (see Figure 30). 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 "Save" function in Part 1 of this user guide).

1	2	4	5	6	7	8
2	ECETOC TRA FLAT DATABASE					
3		1	2	3	4	5
784	Output for Scaling / DU ES Conformity Tool					
785	M_{SPERC} or M_{SITE} (kg/d)	50000	10000	10000	10000	5000
786	Receiving Water Dilution (Fresh or Marine)	10	10	10	10	10
787	Wastewater treatment plant flow (m^3/d)	2000	2000	2000	2000	2000
788	Receiving water body flow rate (m^3/d) [for/alternative to dilution factor]					
789	Optional: Emission days per year	20	10	10	10	20
790	Onsite Removal Efficiency – Air (%)	0	0	0	0	0
791	Onsite Removal Efficiency – Wastewater (%)	FALSE	FALSE	FALSE	FALSE	FALSE
792	Release rate air – after on-site RMMs (kg/day)	2500	250	250	250	5000
793	Release rate wastewater – after on-site RMMs (kg/day)	3000	200	200	200	5000
794	Municipal Sewage Treatment Plant (STP) used ?	yes	yes	yes	yes	yes
795	Municipal Sewage Treatment Plant (STP) removal rate (%)	1.23485242	1.23485242	1.23485242	1.23485242	1.23485242
796	On-site (industrial) Sewage Treatment Plant used ?					
797	Municipal Sewage Sludge applied to soil?	yes	yes	yes	yes	yes
798	Risk Driving Compartment (Code)	1	1	1	1	1
799	M_{SAFE} (kg/d)	6.750019445	20.25005834	20.25005834	20.25005834	0.405001167
800	Risk Driving RCR – Air compartment driven	435.6099256	28.97471272	28.97471272	28.97471272	727.9417626
801	Risk Driving RCR – Water compartment driven	7407.386069	493.8257379	493.8257379	493.8257379	12345.64345

Figure 30: Example output of scaling parameters for environment feeding into a "simple scaling tool" / DU ES Conformity tool as currently developed

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 calculations in the TRA integrated tool are in part made using the copy-paste functions of window and thus the Microsoft Windows clipboard. As such, it is strongly advised to avoid using the copy function, clipboard or Ctrl + C during calculations, as any wrong information being introduce in the tool will cause the Excel sheet to crash. This is even more pertinent when making use of "run batch" as calculation will take more time to finish.

CPU and RAM usage in your PC

The TRA integrated tool is a low demanding tool making use of a single CPU-core and around 100 MB on average of system memory (RAM). However, in certain scenarios the tool may maximize processing power on the loading core resulting in 100 % usage during large batch processes.

This increased CPU usage, depending on the computer's hardware, may cause an overall system slowdown. Using multi-core CPU and closing other resource-intensive programs should reduce computing times and increase system stability during calculations.

Additionally, system memory requirement will increase when inputting large amounts of data, especially when running a large batch process.

Region and language settings of your windows system

Please be aware that the region and language settings of your windows system may have an influence on the operations of the TRA.

Some drop-downs in the Interface include decimal points. In addition, lines 102 and 105/106 of the Datasheets have a drop-down selection for "True" and "False" (for example, the approach you select for the environmental assessment of ERC, SpERC, release fractions, release rates). If your computer uses a different language than English, "True" and "False" will be written in your system's language which may cause issues down the line.

It is important that the display language in excel is set to English (UK). Display language can be changed inside Excel in "Add a Language" if you go into the "Language" options menu (Figure 31 (c)) inside the "File" tab on the top left corner of Excel (Figure 31 (a)) and then the "Options" tab on the bottom left (Figure 31 (b)) ([for more information](#)). Make sure to set English as you 'display language' after the language package is install, if you want to return to your original language after using the tool just select it and click "Set as preferred".

If this does not resolve the issue, you need to change the language and region settings of the entire computer to English (UK) via the Windows control panel.

If you are unable to follow the fixes above a possible workaround is to copy and paste the terms in your computer's language into the fields rather than selecting them from the drop-down menu.
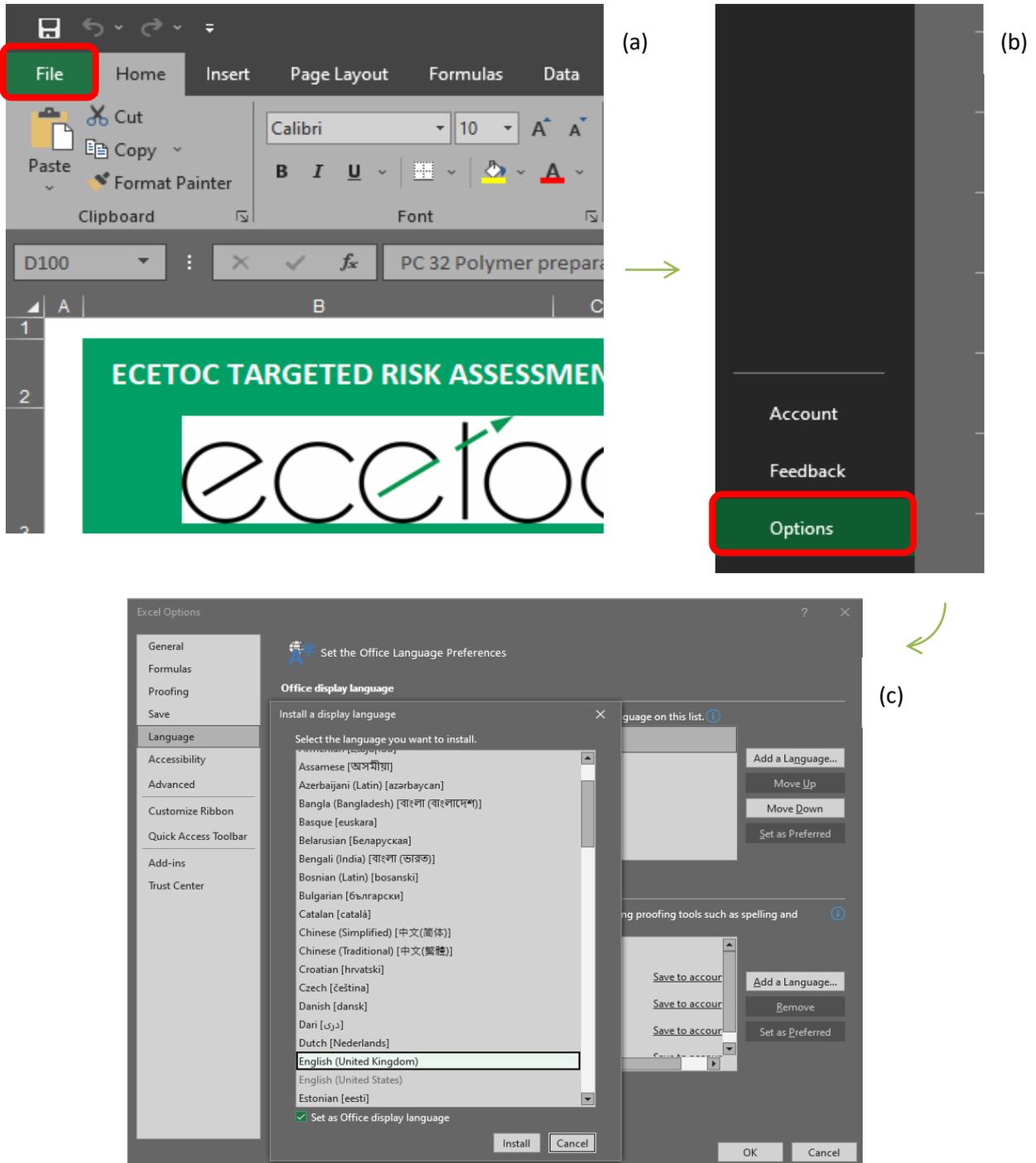
Figure 31. Changing Excel Language

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 (I26) and the end substance number (K26) should be identical, as seen below:

Run batch	Run model using batch mode from database. From substance #	1	to substance #	1

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".

ABBREVIATIONS

AC   Article Category

DNEL   Derived No-Effect Level

EASE   Estimation and Assessment of Substance Exposure model

ECETOC   European Centre for Ecotoxicology and Toxicology of Chemicals

ECHA   European Chemicals Agency

ERC   Environmental Release Category

EUSES   European Union System for the Evaluation of Substances

IND   INDustrial

LEV   Local Exhaust Ventilation

OECD   Organisation for Economic Co-operation and Development

OEL   Occupational Exposure Limit

OC   Operating Conditions

PC   Product Category

PEC   Predicted Environmental Concentrations

PROC   PROcess Category

PROF   PROFessional

PNEC   Predicted No Effect Concentration

REACH   Registration, Evaluation, Authorisation and Restriction of Chemicals

RCR   Risk Characterisation Ratio

RMM   Risk Management Measures

RPE   Respiratory Protective Equipment

SEG   Similar Exposure Group

SpERC   Specific Environmental Release Category

STP   Sewage Treatment Plant

TF   Task Force

TGD   Technical Guidance Documents

TR   Technical Report

TRA   Targeted Risk Assessment

TRAM   Targeted Risk Assessment Model