RELEASE NOTES EU TGD SPREADSHEET VERSION 1.3MS (20080508)

Introduction

This spreadsheet is a multi-species version of the EU TGD spreadsheet version 1.23. It can be used to simultaneously model 5 parent-daughter-granddaughter compounds. Also a regionbase is included, which makes it possible to choose different regions in Northern-America as modeling sites, next to the default region from EUSES. The spreadsheet aims to represent the algorithms described in the 2003-version of the EU Technical Guidance Document, as implemented in EUSES 2.0.3. Although prepared with great care, flawless operation cannot be guaranteed. Comparison of sample calculations with this EU TGD spreadsheet and EUSES 2.0.3 has shown significant differences in some cases. Action is being taken by Industry and European Commission to resolve this. Users of this spreadsheet need to be aware of this. By using this spreadsheet, users accept full responsibility for their calculations. Neither Cefic, nor the producers of this spreadsheet can take liability for (mis)use of the results. This spreadsheet can be obtained free of charge from the Radboud University Nijmegen (www.ru.nl/environmentalscience), Free University (www.bio.vu.nl) and Cefic (www.cefic.org). Distribution of the spreadsheet to third parties is allowed only with permission of Cefic.

Observed differences between EU TGD spreadsheet and EUSES

This spreadsheet is meant to implement the risk assessment algorithms described in the EU Technical Guidance Documents. The spreadsheet was prepared with care, and tests were run against EUSES 2.0.3. Differences observed during these tests have revealed errors in the spreadsheet code, which have been corrected. A number of the observed points of difference have remained unresolved. Further research is planned to resolve these. This is to inform users of the observed differences:

1. **Vapor pressure of the liquid phase (*VP.L*), and Henry's law constant (*HENRY*)**

It is believed that EUSES and the spreadsheet interpret the TGD differently with respect to temperature corrections implemented. This can lead to differences in the values of *VP.L* and *HENRY*. It is recommended that users verify if their preferred values are used in the calculation.

2. **Volatilization from soil (*k.volat.agric*, *k.volat.grass*)**

It is believed that EUSES has a different implementation of equation 159 of Lijzen and Rikken (2004). We noticed that EUSES keeps using the parameters *kas.soilair* and *kasl.soilwater*, which are not defined in the recently implemented version of SimpleBox. In critical situations, users are recommended to check this manually.

3. **Local concentrations in sea water**

It seems that EUSES emits raw sewage to the marine water, whereas the spreadsheet emits STP-effluent. Users are recommended to check this manually and correct where necessary.

4. **Regional distribution**

EUSES reports different residence times (air at moderate scale, sea water at regional and continental scales) and sedimentation rates (notably sea water at the continental scale) that differ from the residence times used by the spreadsheet. Without further in-depth study, no recommendation can be given to this end.

5. **Assessment factors**

Default assessment factors for the human effect assessment in the spreadsheet follow the recommendations given in the TGD, whereas EUSES applies assessment factors of 1 by default. Users are recommended to make their own choice here.

Guidance for users

Concept of the EU TGD spreadsheet

Calculations in this spreadsheet are performed with the original spreadsheets of SimpleBox 3.21ms, a multi-species version of SimpleBox 3.0 (Den Hollander *et al.*, 2004), and SimpleTreat 3.1 (Struijs, 1996). These spreadsheet models are linked to the EU TGD spreadsheet and loaded automatically upon opening the EU TGD spreadsheet. To be able to run the EU TGD spreadsheet, sbtools.xla has to be installed **in the folder C:\program files\sbtools**. The risk assessment algorithms from the EU Technical Guidance Documents, as described by Lijzen and Rikken (2004), are coded on a number of different worksheets within the EU TGD spreadsheet.

As a service to regular users of EUSES, the calculation flow of EUSES 2.0 is followed closely.

- Identical parameter entry headings are used in EUSES and the EU TGD spreadsheet
- On the worksheets, variables appear in the same order as they do in EUSES
- Variables in the spreadsheet are named after variables in Lijzen and Rikken (2004).

- Names of the variables of the 2nd, 3rd, 4th, and 5th substance are completed with .beta, .gamma, .delta, and .epsilon, respectively
- Variables that are equal for all species only appear in the column of the alpha-species
- Model input values applied and model outputs produced from it are reported (worksheet "report") in the same order as they appear in reports produced from EUSES.
- For easy use, the worksheet "in&out" has been created. This worksheet lists the most frequently set model inputs and the most frequently consulted model outputs. For most routine risk assessment calculations, working on the "in&out" worksheet should suffice.

Risk assessments are carried out by entering the necessary model input values. Each time a value is entered or changed, the entire system of spreadsheets is recalculated automatically, updating all model outputs. Upon completion of the process of entering input data, model outputs are ready for use; no further action by the model user is necessary.

Protection

The EU TGD spreadsheet and its supporting spreadsheet models are 'read only' to prevent unintentional override of the original models. Work is to be saved as a copy of the original spreadsheet. In addition, all spreadsheet cells have been locked, except those designed to receive user input. No password protection of the spreadsheet locking has been set, to allow advanced users to unlock the spreadsheet. Unlocked cells, to which user input is allowed, fall in different categories, indicated with different background colors:

- Pale yellow. Cells designed to accept user input in routine operation. Such cells are located on the "in&out" worksheet only.
- Light grey. Cells designed to accept user input in advanced user operation. Such cells can be found on the regular model input worksheets. By entering numbers into these cells specific models can be formulated by changing default options. Recommended for advanced users only.
- Dark grey. Cells open to accept expert user input in exceptional cases only. Recommended for modeling experts only.

Operation

- Store the original files in a safe place.
- Make working copies of the five EU TGD files ('EUTGDsheet1.3MS.xls', 'SimpleBox 3.21ms.xls', 'SimpleTreatL.xls', 'SimpleTreatR.xls', 'SimpleTreatC.xls') in one directory.
- Open the spreadsheet 'EUTGDsheet1.1aMS.xls'. The supporting spreadsheet models 'SimpleBox 3.21ms.xls', 'SimpletreatL.xls', 'SimpletreatR.xls' and 'SimpletreatC.xls' are opened automatically.
- Make sure that the box 'sbtools' is checked under the Excel menu 'Tools|Add-Ins'.
- If you anticipate later consultation or continuation of your work, save the working copy of EUTGDsheet1.3MS.xls under a new name, using the Excel menu 'File|Save as'
- Enter input data into the appropriate cells of the EU TGD spreadsheet. For routine use, entering data into the pale yellow cells on the worksheet 'in&out' (column E-I, rows 11 - 338) should suffice.
- For calculating the steady-state model output, press the button at the top of the in&out sheet
- Read steady-state results (concentrations, daily intake, no effect levels, ecosystem risks and human risks) from the green cells on the 'in&out' worksheet (Columns E-I, rows 345 -530).
- An extensive report of the risk assessment, similar to the reports produced from EUSES, can be read or printed from the worksheet 'report'.
- To perform a dynamic calculation, set the appropriate parameters on the worksheet 'dynamic input' and press the button at the top of that worksheet.
- Results of the dynamic calculations can be read from the 'dynamic output' worksheet
- Use the Excel menu 'EU TGD spreadsheet|Save and exit' to save your work. In doing so, adjusted copies of 'SimpleBox 3.21ms.xls', 'SimpleTreatL.xls', 'SimpleTreatR.xls', 'SimpleTreatC.xls' are written in your work directory, which will be re-opened upon re-opening the working copy of your EUTGDsheet.

Error messages

It is possible that, when opening the spreadsheets, an error message occurs. This is what you should do:

- 'This file contains macro's' -> choose 'enable macro's'
- 'Macro's in this workbook are disabled' -> Go to 'tools' – 'options' – 'security' – 'macro security' and set this on medium or low.

Literature

1. H.A. den Hollander, J.C.H. van Eijkeren and D. van de Meent. SimpleBox 3.0. RIVM report 601200003/2004
2. J. Lijzen and M. Rikken (eds.). EUSES 2.0 Background Report. RIVM Report no. 601900005/2004
3. J. Struijs. SimpleTreat 3.0: a model to predict the distribution and elimination of chemicals by sewage treatment plants. RIVM report no. 719101025/1996