



EasyGUTS Running R GUTS scripts in a Windows® based software

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SUMMARY

We developed a Windows® software to manipulate and run R GUTS scripts for the evaluation of surface water exposure profiles calculated with the environmental fate model FOCUS TOXSWA 4.4.3. One of the modelling tools in higher tier aquatic risk assessments can be the toxicokinetic and toxicodynamic General Unified Threshold Model of Survival (GUTS), which is similar to body burden modelling approaches in higher tier wildlife risk assessments. However, the first published GUTS version was written in R, a command-line program using its own script programming language, which is difficult to use for those who are not familiar with R. Therefore, we developed a user-friendly Windows® program in the modern programming language VB.Net, which can run GUTS R scripts for parameterisation and validation of aquatic laboratory tests. Moreover, we implemented an additional functionality, which links the outcome of GUTS with exposure files from the environmental fate model TOXSWA. The user can then easily extract the exposure profiles from TOXSWA text output files and perform a moving time window analysis to evaluate potential worst case exposure profiles.

INPUT DATA

EasyGUTS requires two kinds of input data:

• Effect data:

Survival data and effect concentrations over time stored in text file format like .csv file (a data row consists of concentrations, time of concentration measurements, number of survivors, time of survivor measurements)

• Exposure files:

Exposure profiles like TOXSWA output files (.out) containing concentration values over time (see Figure 1)

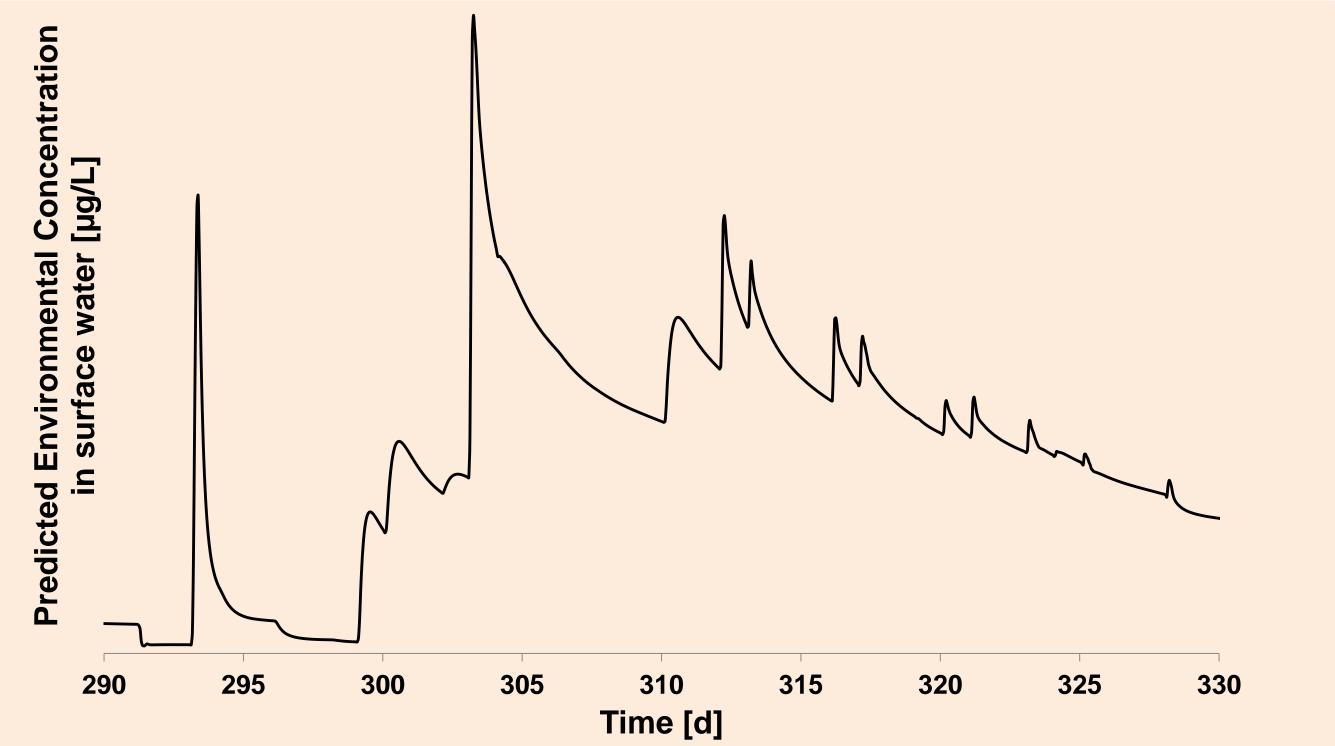


Figure 1: Exposure profiles calculated e.g. with FOCUS-TOXSWA 4.4.3

FUNCTIONALITIES

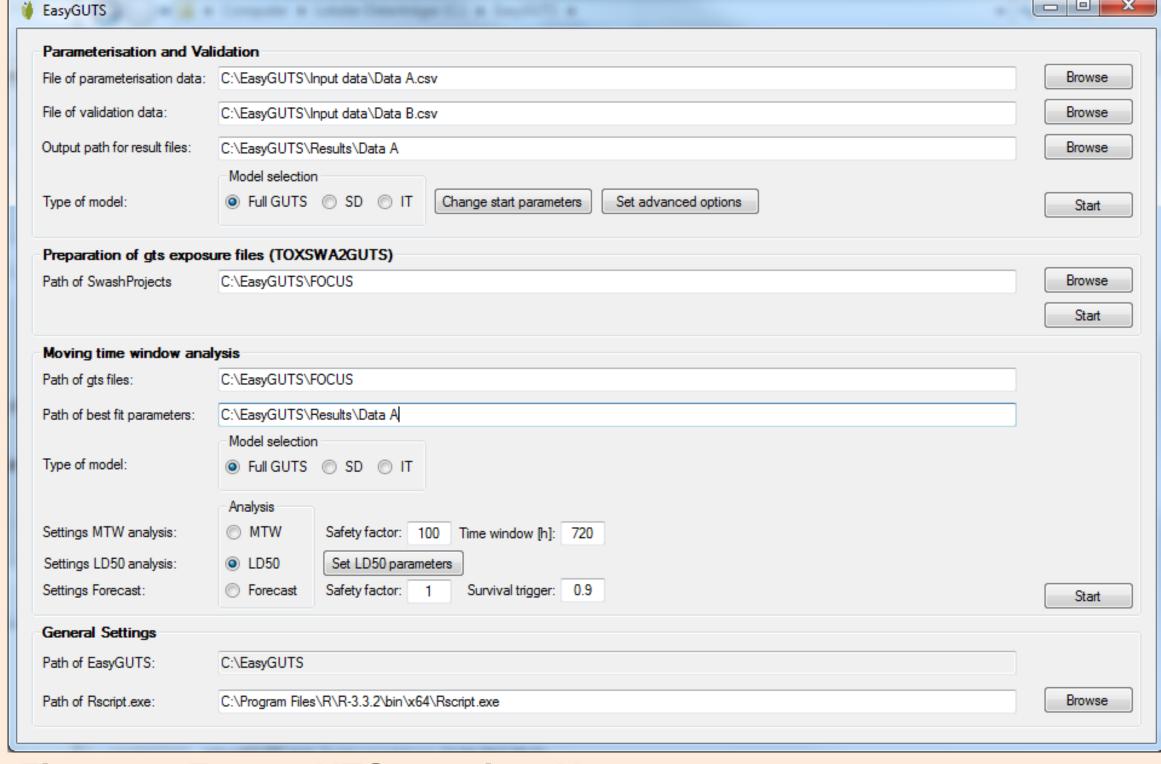


Figure 2: Easy-GUTS's main GUI

EasyGUTS provides three main functionalities:

- Parameterisation and validation of GUTS:
 Evaluation of survival toxicity tests; optimisation of
 parameters was implemented according to Albert et. al.
 2016 (Hooke-Jeeves, MCMC analysis)
- Preparation of exposure files:
 Extraction of exposure profiles from TOXSWA .out files (parameter 'ConLiqWatLayCur', last compartment)
- Analysis:

Survival analysis like moving time window analysis of all available exposure profiles or LC50 calculations

OUTPUT DATA

EasyGUTS offers a variety of output options in graphical and text form:

- Overview of model parameters (best fit, user defined quantiles)
- Descriptive statistics of model parameters
- Survival rates
- LC50 values
- Worst case exposure profiles

