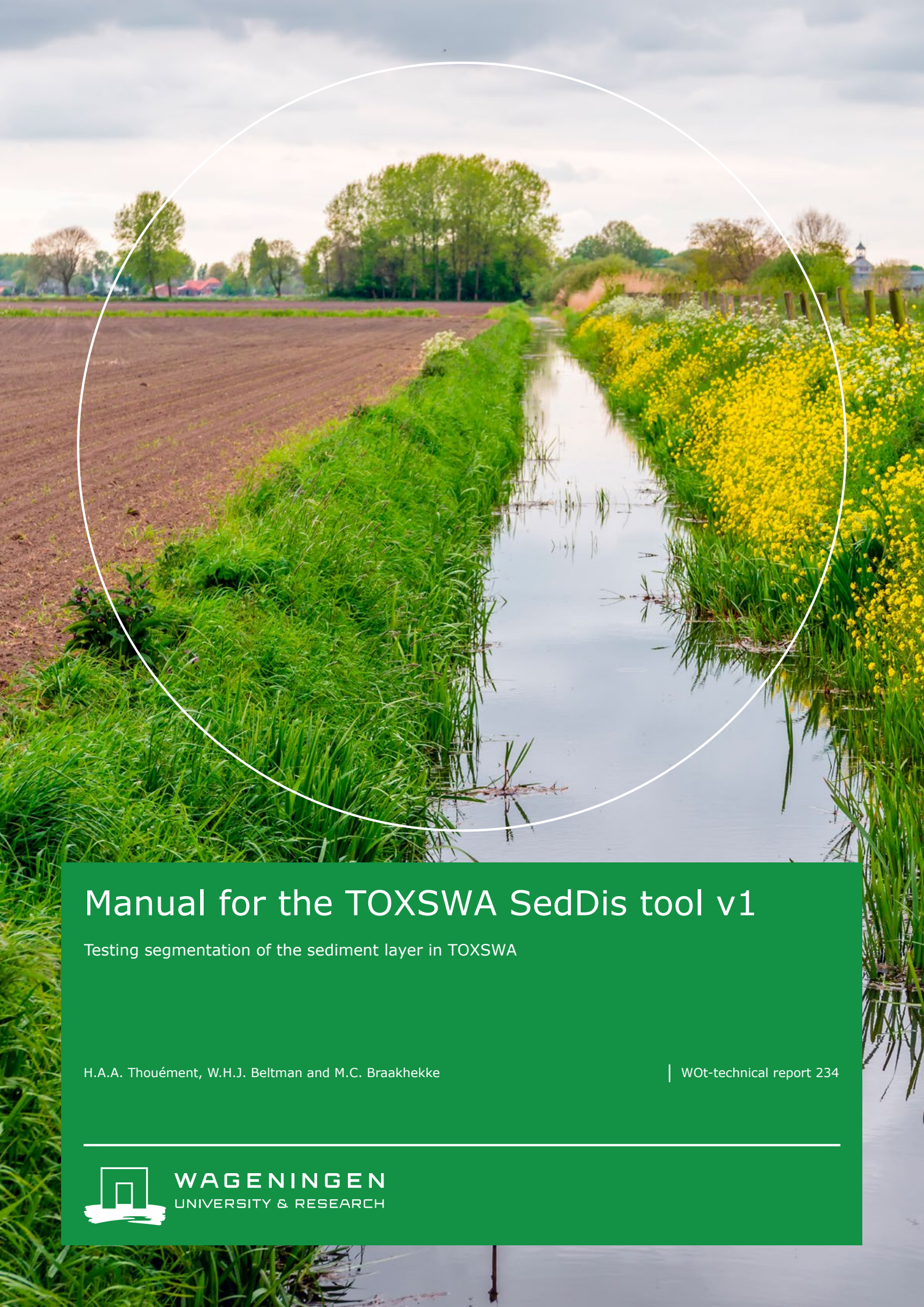

Manual for the TOXSWA SedDis tool v1

Testing segmentation of the sediment layer in TOXSWA

H.A.A. Thouément, W.H.J. Beltman and M.C. Braakhekke

WOt-technical report 234

WAGENINGEN
UNIVERSITY & RESEARCH

Manual for the TOXSWA SedDis tool v1:

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Abstract

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The SedDis tool is a decision-support tool for selecting the optimal segmentation for the sediment in TOXSWA simulations. The TOXSWA model is used to calculate exposure concentrations of pesticides and their metabolites in watercourses and ponds. For the parameterization of the water body, its water layer and sediment layer need to be spatially discretized. For the sediment layer, the size of the grid (segmentation) is crucial. Selecting the optimal segmentation ensures that simulated concentrations are calculated with a satisfying accuracy when simulating the transport of strongly sorbing compounds within the TOXSWA model. The theoretical background and methodology for the SedDis tool is described. The procedure for using the SedDis tool is provided. Instructions for running the tool with an example (selecting standard or fine segmentation for a given scenario) are given.

De SedDis tool is een beslissingsondersteunend instrument voor het selecteren van de optimale segementatie voor het sediment in TOXSWA-simulaties. Het TOXSWA-model wordt gebruikt om blootstellingsconcentraties van pesticiden en hun metabolieten in vijvers en waterlopen te berekenen. Voor de parameterisatie van het waterlichaam, worden de waterlaag en sedimentlaag ruimtelijk in segmenten verdeeld. Voor het sediment is de segmentatie cruciaal. Het selecteren van de optimale segmentatie zorgt ervoor dat de blootstellingsconcentraties met een acceptabele nauwkeurigheid worden berekend voor sterk adsorberende stoffen. De theoretische achtergrond van de methode wordt beschreven, en ook de installatie en procedure voor gebruik van de tool. Instructies voor het gebruik van de tool met een voorbeeld – selectie van een standaard segmentatie of fijnere segmentatie voor een gegeven scenario – worden gegeven.

Keywords: model, sediment, segmentation, segment thickness, spatial discretisation, pesticide.

Photo cover: Shutterstock

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Preface

A Python tool to test the optimal segmentation of the sediment used by the TOXSWA model was developed by Niamh O' Connor (now University of Sheffield, UK), Louise Wipfler, and Wim Beltman. We thank Louise Wipfler for her preliminary work, and for selecting and describing the appropriate method for this tool. The tool has been improved and made more error prone by Héloïse Thouément and Maarten Braakhekke. Héloïse Thouément added an Excel sheet to summarize and present results of a test. The tool works with TOXSWA version 3.3. This manual is a first version.

Contents

Summary

This user-guide describes the Sediment Discretisation software package (SedDis). This package contains a decision support tool that was developed for selecting the optimal segmentation for the sediment in TOXSWA simulations.

When simulating transport in numerical simulations, for instance, the transport of strongly sorbing compounds in sediments, the segmentation employed influences the results of the simulation. Refining the segment thickness improves the simulation quality but increases the computational time. We recommend to evaluate which segment thickness to use for obtaining a result with a satisfying accuracy, i.e. when the simulation is not improved (compared to an acceptable error) with a smaller segment thickness. This manual addresses the clear need for a scientifically underpinned and pragmatic approach towards the setting of this segmentation in the TOXSWA model, as used in the risk assessment context, and is attached to a tool promoting the use of this approach.

The methodology used in this tool is based on the so-called, 'Richardson extrapolation'. Furthermore, this tool facilitates the construction of the input files, parallel running of the simulations, and the extraction of the simulation results (exposure concentrations in water) from the different output files. A pre-filled Excel sheet is provided to calculate the parameters of the Richardson extrapolation. Instructions are given on how to obtain and interpret the parameters of the Richardson extrapolation for one example. Subsequently, instructions are provided on how to determine those parameters for your own simulation.

Samenvatting

Deze handleiding beschrijft het Sediment Discretisation software-pakket (SedDis). Dit pakket bevat een beslissingsondersteunend instrument dat ontwikkeld is voor het selecteren van de optimale verdeling van segmenten in het sediment ten behoeve van het oplossen van de numerieke vergelijkingen in TOXSWA-simulaties.

Wanneer transport van stoffen wordt gesimuleerd met numerieke berekeningen, bijvoorbeeld het transport van pesticiden en metabolieten in sediment, kan de gebruikte verdeling van de segmenten in het sediment invloed hebben op de resultaten. Verfijnen van de segmentatie verbetert de kwaliteit van de simulatie, maar leidt ook tot een langere rekentijd. We adviseren om een segmentatie te gebruiken die resultaten geeft met voldoende nauwkeurigheid, d.w.z. als de simulatie niet is verbeterd (vergeleken met de acceptabele fout) met een fijnere segmentatie. Deze handleiding voorziet in een wetenschappelijk onderbouwde en pragmatische aanpak om segmentatie te selecteren voor het TOXSWA-model, gegeven de context van het gebruik van TOXSWA in de risicobeoordeling van blootstelling van waterorganismen in oppervlaktewater. De handleiding beschrijft ook het gebruik van een instrument om de beschreven aanpak toe te passen.

De methode die is toegepast in het instrument is gebaseerd op de zogenoemde Richardson-extrapolatie. De tool faciliteert het maken van invoerbestanden, parallel rekenen van de simulaties, en het samenvoegen van resultaten (blootstellingsconcentraties in water) uit de verschillende uitvoerbestanden. Een vooraf ingevuld Excel-rekenblad waarmee de parameters van de Richardson-extrapolatie kunnen worden berekend is meegeleverd. Er worden instructies gegeven voor hoe de resultaten kunnen worden verkregen en hoe de parameters kunnen worden geïnterpreteerd. Dit is toegelicht aan de hand van een voorbeeld. Daarnaast worden instructies gegeven voor hoe de parameters kunnen worden verkregen voor een eigen simulatie.

1 Introduction

This document describes a decision support tool which can be used to select an appropriate sediment segmentation for simulations with TOXSWA (TOXic substances in Surface Waters). For simulation with TOXSWA the sediment layer is divided in a regular series of contiguous segments, with thinnest thickness below the water layer, and greater thickness below. Refinement of the sediment segmentation (= segment thicknesses, i.e. sediment discretisation) is sometimes needed to reduce the numerical error, while solving the conservation equation. In view of the sensitivity of the model to the sediment segments thicknesses and its impact on the calculation time, there is a need for a scientifically underpinned and pragmatic approach towards the setting of this segment thickness in the TOXSWA model, as used in the risk assessment context. Decision-making on the optimal segments thicknesses/segmentation is currently performed on a case-by-case basis, i.e. the optimal segmentation is derived for each application. Hence, for TOXSWA, applied segments thicknesses in the FOCUS_TOXSWA application and TOXSWA in the GEM application differ, due to differences in sediment properties and flow velocities. This report aims to provide guidance and background on a standard procedure on how to assess the discretisation error and when to reduce the segment thickness of the sediment.

The SedimentDiscretisation (SedDis) tool consists of a Python script and an Excel-based tool. The Python script automatises the creation of TOXSWA input files for the chosen sediment segments thicknesses and K_{om} values, automatises parallel running of the simulations, then extracts the Predicted Environmental Concentration (PEC) values for surface water from the TOXSWA summary files. Those data have to be copied to the Excel-based tool, which provides the necessary calculations for the interpretation of the results and a graphical report.

The decision-support tool presented in this User guide is intended for use by expert users. The tool allows comparison of the convergence of the simulations obtained with the standard segmentation *versus* the fine segmentation provided in the TOXSWA simulations. It also enables identification of whether further segmentation refinement could improve the results accuracy. The methodology used is based on the so-called, 'Richardson extrapolation'.

2 When to use the SedDis tool

The SedDis tool is intended for use as a decision support tool for TOXSWA developers and for expert users of TOXSWA to define the appropriate segment thickness in the sediment compartment. In the current TOXSWA applications (e.g. FOCUS_TOXSWA and GEM), two segmentations are available for simulations. The segmentation used for the simulation is selected based on the sorption coefficient of the tested substance. In the TOXSWA application, the setting switches automatically from a standard sediment segmentation to a finer sediment segmentation when the sorption coefficient is above a certain value. For instance, in GEM scenarios, for sorption coefficients < 1000 L/kg, the standard segmentation is used, while for sorption coefficients larger than 1000 L/kg, the finer segmentation is used. For FOCUS and DRAINBOW, the value at which the switch between the two segmentations is set is 30 000 L/kg, based on tests, in which results for the two segmentations were compared. The switch values differ due to differences in sediment properties and flow velocities of water in the waterlayer.

Although the automatic switching between segmentations as described above works in standard cases, it is recommended to use the SedDis tool for testing if the segmentation is appropriate:

- When a scenario is developed that includes two or more sediment segmentations to determine the sorption coefficient at which a switch should be made between segmentations.
- To check if a segmentation gives sufficient accurate PEC for a certain sorption coefficient. For instance, when the sorption capacity of a parent and a metabolite differ. A very mobile compound cannot be simulated with a fine segment thickness, while it is common to simulate a mobile parent compound and a less mobile metabolite, in which case different segments thicknesses can be necessary[1].
- For molecules with large sorption coefficient (>100 000 L/kg), as PEC concentrations might be overestimated. The tool can help evaluating the existing error and quantify the accuracy gain with segments thicknesses refinement.

This SedDis tool should be seen as a decision-support software tool for selecting the appropriate segments thicknesses in the sediment compartment. The tool automatizes input file creation and results (predicted exposure concentrations in surface waters) extraction, but it should not be considered as a ready-to-use tool. The tool provides you with example input files for the discretisation selection and shows you how to interpret the results. The user is responsible for correctly defining the input files that correspond to a specific case-study and also the interpretation of the results.

The SedDis tool does not take formed metabolites into consideration. The simulation for a metabolite should be performed with the metabolite modelled as a parent compound.

[1] Sometimes a parent and its metabolites can have sorption coefficients on both sides of the switch value. E.g. the parent has a sorption coefficient that can be run with the standard segmentation and the metabolite a sorption coefficient that should be run with the fine segmentation. The run can be done with the fine segmentation, because this gives accurate values of PEC for both parent and metabolite. However, in some cases TOXSWA cannot run the low sorption coefficient of the parent with the fine segmentation due to numerical reasons. In this case, TOXSWA can run the high sorption coefficient of the metabolite with the standard segmentation. SedDis can, in such a case, be applied with the metabolite sorption coefficient to determine the accuracy of the PEC of the metabolite for the standard segmentation. That is, the segmentation that was not meant to be used for the metabolite's sorption coefficient. On the other hand, when the PEC of a metabolite is a trigger in the risk assessment, other work-ups need to be used.

3 Background

3.1 TOXSWA simulation model

The pesticide fate model TOXSWA is a pseudo-two-dimensional model that describes pesticide behaviour in a water layer and its underlying sediment at the edge-of-field scale (Adriaanse, 1996). TOXSWA calculates Predicted Environmental Concentrations (PECs) in surface water for the environmental risk assessment of pesticides. TOXSWA is currently part of several exposure assessment instruments in use, e.g. FOCUS-TOXSWA, GEM and PRIMET-Ethiopia.

TOXSWA simulates pesticide fate in water bodies, such as ditches and ponds. Processes simulated include advection and dispersion in the water phase, exchange with the atmosphere through a diffusive flux, exchange with the sediment through an advective and diffusive flux, adsorption to sediment and suspended particles, degradation in the water phase and in the sediment (Adriaanse, 1996; Ter Horst et al., 2016). Figure 1 shows the diagram of the simulated processes, as given in Adriaanse (1996).

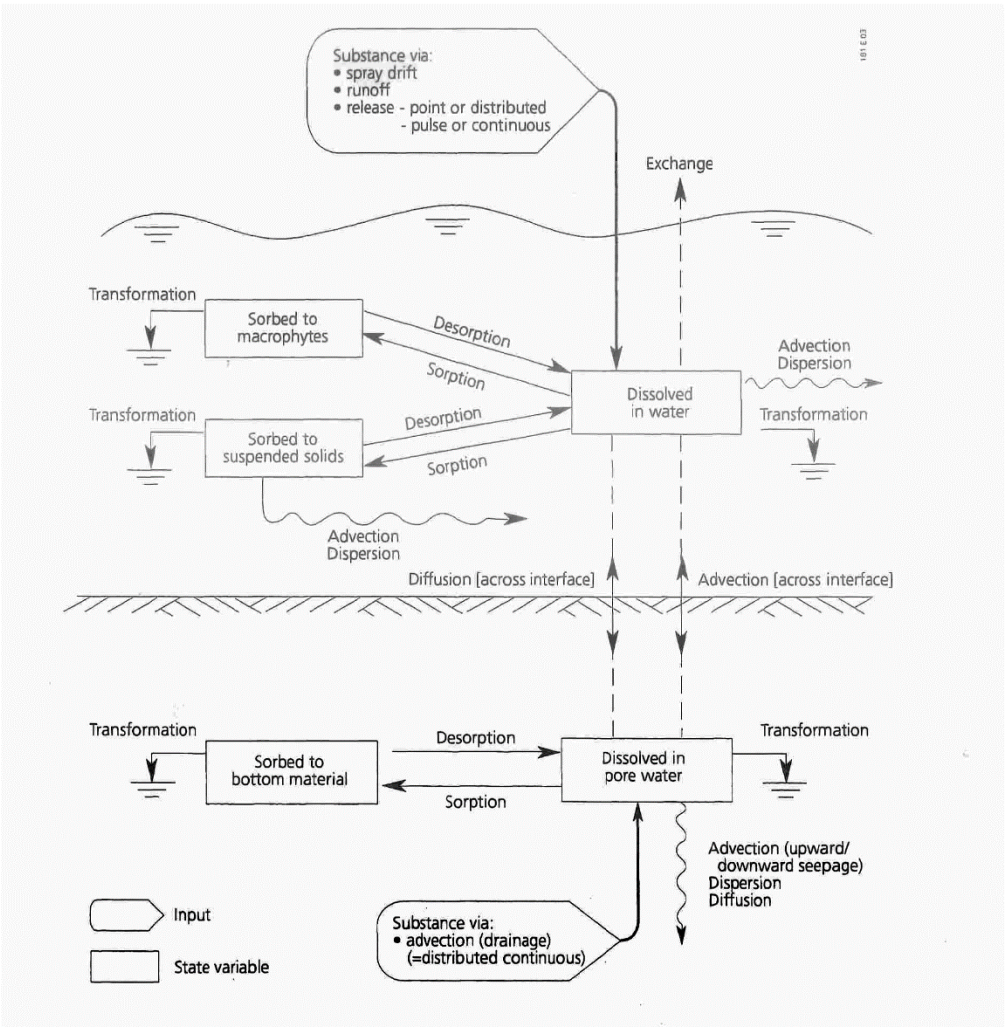

Figure 1 *Simulated processes by TOXSWA (from Adriaanse, 1996).*

The ditch system, as simulated by TOXSWA consists of two subsystems: the water-layer and the sediment. These subsystems exchange water and pesticide mass via diffusion over the so-called 'wetted perimeter' of

the water body. The model solves the conservation equations for both the water layer and the sediment system numerically. This is done by dividing the water body into several connected water layer segments with a sediment subsystem that is also divided in segments for each water layer (Figure 2). For the model results to converge, the segments are thinnest at the boundary with the water layer. The sediment layer configuration is the same for each of the water segments.

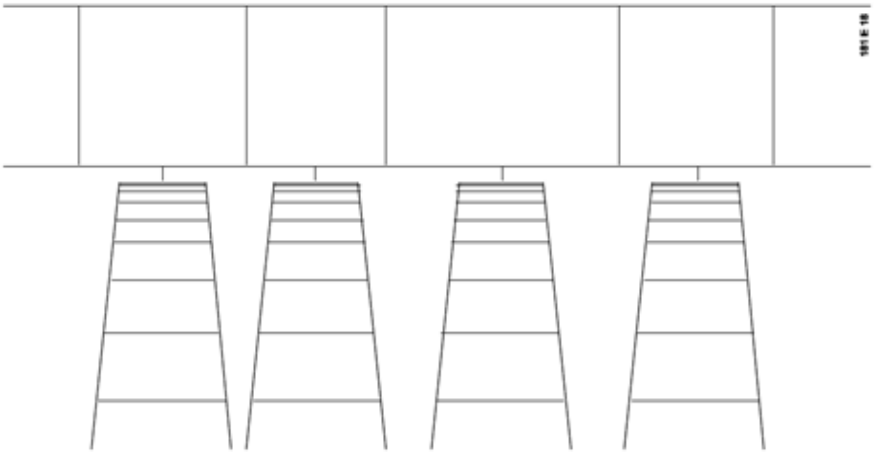

Figure 2 *Structure of the TOXSWA water body system. One water layer subsystem (top, horizontal) and many sediment subsystems (bottom, trapezoidal) (from Adriaanse, 1996). The segment thickness studied here concerns the different sediment subsystems. Each is connected to a water layer but there is no transfer between the sediment subsystems.*

Refinement of the sediment segments thicknesses is sometimes needed to reduce the numerical error while solving the conservation equation. For example, in case the adsorption potential of the simulated substance increases the (vertical) segment thickness of the sediment layer needs to be refined. This introduces larger calculation times. The model appears to be very sensitive to the sediment segment thickness for strongly adsorbing pesticides (Deneer et al., 2014).

3.2 General approach of the segmentation convergence study

The TOXSWA model solves the conservation equation of pesticides by using a forward differencing finite difference scheme for both the water layer as the sediment compartment(s). The associated discretisation error is defined as the difference between the exact/real solution, obtained through a convergence study, and the numerical solution. When the segmentation is refined (denser segmentation, i.e. the number of segments increases) the spatial discretisation error should approach zero, excluding the computer round-off error. This signifies that when the simulation results are accurate within an acceptable error, a denser segmentation will not result in a significantly different solution. A segmentation convergence study (also found in the literature as "grid refinement study") provides insights in the relation between segmentation and numerical error and can consequently support the optimal segmentation selection. The method used in this tool is a method popular in computational fluid dynamics (CFD) for examining the spatial and temporal convergence of CFD simulations is based on the Richardson's extrapolation. A summary of the method is presented in Section 3.3.

The method applied in the provided tool consists of the following steps:

- Run the model three times with consecutive refinements of the tested segmentation and obtain the result value on which the convergence will be tested (here, on the predicted exposure concentration values (PEC)).
- Based on the three simulations results, calculate the result value (here, PEC) for the segments thicknesses approaching zero ($f(h \rightarrow 0)$, i.e. the limit value of the result (f) when the segments thicknesses (h) is reaching 0, or continuum value $f_{h=0}$) using the Richardson extrapolation approach (see Section 3.3).

- Define the acceptable relative convergence error, i.e. the range within which the simulated value will still have a meaning for the purpose of the simulation. The acceptable size of the numerical error depends on the context and the model. In the case of the estimation of PEC values, an error of 2% was deemed acceptable.
- Compare the results of the simulations to the asymptotic solution $f(h \rightarrow 0)$ and compare their difference to the acceptable error to determine an acceptable segmentation.

One requirement is that the segmentation refinement is within the asymptotic range of convergence, i.e. the results approach the asymptotic value when the segments thickness is smaller[2]. Given that the TOXSWA model has been applied and has converged well (Adriaanse, 1996), a formal check on the convergence of the model given the generally used refinement is not considered necessary.

3.3 Theoretical background of the segmentation convergence study

The procedure for optimized segmentation is based on a method that is popular in Computational Fluid Dynamics and is described in Roach (1994). A summary of this approach is accessible online (Examining Spatial (Grid) Convergence (nasa.gov)). In this theory, the term "grid" is used while we prefer to use segmentation in our report, as the sediment is segmented over one dimension and the term is commonly used with TOXSWA. Note, that the sediment layer is not divided in segments of equal thickness as presented in Section 3.1.

In this theory, the value of the studied parameter for the segments thicknesses approaching zero, also called the continuum value $f_{h=0}$, is calculated via simulation results that were obtained from two or more different segmentations. In the present study and the provided tool, the simulation results were performed for three segmentations. The continuum value is a value that belongs to a segmentation in which segment thickness is infinitely small. The equation for the continuum value and equations for characterizing the segmentation convergence are given in this section. Using the Richardson extrapolation, the continuum value, $f_{h=0}$, is calculated (assuming $f_1 < f_2$) with:

$$f_{h=0} \cong f_2 + \frac{(f_1 - f_2) r^p}{r^p - 1} \qquad (1)$$

With

$f_{h=0}$ = continuum value of the studied parameter.
f_1 = result value for 1st order segment thickness, obtained through simulation.
f_2 = result value for 2nd order segment thickness, obtained through simulation.
r = grid refinement ratio.
p = order of convergence.

In this study, the parameter we examined (f) was the predicted exposure value (PEC) value for surface water (PECsw). Note, that the PEC for sediment could have been compared as well[3]. A segmentation refinement ratio of 2 was applied and is the same ratio between the segmentation G1 and G2 and the segmentation G2 and G3; hence $r = 2$.

[2] Note, that strong divergence from the asymptotic value can relate to the year at which the PEC value occurs. When, e.g., the 90-percentile year for f_1 is 1980, and for f_2 it is 1985, the PEC values will then not be comparable. The history of PEC values in different years differs, and for different segmentations, the percentile year selected may change. The PEC years and PECs can be found in the summary file ('.sum') that can be found in the result simulation folder (for instance, SedDis/1000/f1).

[3] Instead of the PEC in water, the PEC in sediment (PECsed) can also be tested. PECsed is calculated across a certain thickness of the upper part of the sediment. For instance, in the FOCUS scenarios, this thickness is set to 5 cm. This thickness must correspond to the sum of existing consecutive segments in the sediment. While the fine segmentation (f_1*) and the standard segmentation (f_1) allow for this, there is no combination of the upper layers thicknesses in the rougher segmentations f_3, f_2* and f_3* summing to exactly 5 cm. The PECsed can be compared only by choosing a thickness that can be set for all segmentations, as close as possible to 5 cm.

The order of convergence is calculated from three segmentation refinement steps with:

$$\boldsymbol{p} = \frac{\ln\left(\frac{\boldsymbol{f_3} - \boldsymbol{f_2}}{\boldsymbol{f_2} - \boldsymbol{f_1}}\right)}{\ln(\boldsymbol{r})} \tag{2}$$

Where:
f_3 = value for 3rd order segmentation

When the continuum value has been calculated, the fractional error *A* for each of the *f*-values can be calculated with:

$$\boldsymbol{A_1} = \frac{\boldsymbol{f_1} - \boldsymbol{f_{h=0}}}{\boldsymbol{f_{h=0}}} \tag{3}$$

From the above results, it is possible to determine if the results are within an acceptable error range through evaluating the Grid Convergence Index (*CGI*) which provides a consistent manner to report segmentation convergence (or segmentation refinement) studies. The parameters calculated in the following enable the evaluation of the *CGI*:

The relative error between the result from the second discretisation (f_2) and the first (f_1), ε_{21}, is defined as:

$$\boldsymbol{\varepsilon_{21}} = \frac{\boldsymbol{f_2} - \boldsymbol{f_1}}{\boldsymbol{f_1}} \tag{4}$$

The *GCI* is a percentage measure that indicates how far the computed value is from the asymptotic numerical value. It indicates an error band on how far the solution is from the asymptotic value and how much the solution would become more accurate with a further refinement of the segmentation. The *GCI* on the fine segmentations (here f_1 segmentation) is defined as:

$$\boldsymbol{GCI_{21}} = \frac{\boldsymbol{F_s}\,|\boldsymbol{\varepsilon_{21}}|}{\boldsymbol{r^p} - \boldsymbol{1}} \tag{5}$$

where F_s is a factor of safety. The factor of safety is recommended to be F_s **=** 3.0 for comparisons of two segmentations and F_s **=** 1.25 for comparisons over three or more segmentations (this case). Calculations for the *CGI* for the coarser segmentation refinement (f_2) are available in the literature.

The *CGI* provides a consistent manner in reporting the results of segmentation convergence studies and also provides an error band on the solution's segmentation convergence.

4 Installing the SedDis tool

The SedDis tool is distributed in a zip file ('SedDis_tool.zip').

The software package consists of:
- A Python script (SedDis_tool.py).
- An Excel spreadsheet (SedDis_Output_Interpretation.xlsx) for calculating the parameters (based on the Richardson extrapolation) allowing to evaluate the segmentation refinement.
- The input files necessary to run an example (folder 'SedDis_tool_example_1', see Section 5.3.1).

To run the tool a Python interpreter is required, which can be obtained from https://www.python.org/downloads/. Additionally, several Python packages are required. These are specified in the file requirements.txt. The packages can be installed using the Python package manager pip. Pip is typically included with the Python interpreter. If not, it can be obtained from: https://pip.pypa.io/en/stable/installation/.

Hence the steps are:
1. Download the zip file ('SedDis_tool.zip').
2. Unzip the file and specify a path (e.g. D:\Sediment_discretisation). Ensure that there is no space within the specified path because this will cause failure of the TOXSWA simulation.
3. Check if pip is present by running in the command prompt command line: "`python -m pip --version`", if not download and install.
4. Using the command prompt, run in command line from the folder 'SedDis_tool': "`pip install -r requirements.txt`".

You are now ready to start using the SedDis tool.

5 Description of folder structure and files of the SedDis tool

5.1 Introduction

The SedDis Python script processes three steps:
1. It creates the input files for a number of different sediment segmentations and different sorption (partition) coefficient to organic matter K_{om} values.
2. It runs the TOXSWA simulations.
3. It extracts the PEC values from the TOXSWA summary files and stores these in a .csv file.

Before running the script, the user needs to ensure that the folder structure is set up correctly and the appropriate files are available. In this Chapter, the folder structure, file overview and description of files is given.

5.2 Folder structure

All files for running the SedDis tool can be found in one folder. The user can choose the name of the main folder (here in the example 'Simulation'). In this main folder is one folder ('SedDisFiles'), itself containing a second folder ('TOXSWA_Inputs'). The files contained in those folders are presented in the following sections. The folder structure before running the tool is the following:

Example Folder structure:

Simulation	Folder with name chosen by the user
└── SedDisFiles	Input data directory
├── f1.inp	Discretisation file (standard and fine)
├── f1std.inp	
├── f2.inp	
├── f2std.inp	
├── f3.inp	
├── f3std.inp	
├── ref.txw	TOXSWA template input file
├── TOXSWA_SedDis.inp	SedDis input file
├── toxswa.exe	TOXSWA executable
└── TOXSWA_Inputs	Folder with additional input files
├── toxswa.met	Meteorological file
└── (.g2t/.s2t/...)	Scenario specific files

5.3 Overview of input and output files

5.3.1 Input files

The python script ('SedDis_tool.py') prepares the folder structure and the input files for the TOXSWA simulations.

The Python script needs three types of files (see details in Table 1):
- Files specific to the SedDis tool, needed in input folder ('SedDisFiles').

- Files commonly required for all TOXSWA simulations, e.g. meteo file ('.met'), needed in input folder 'SedDisFiles\TOXSWA_inputs', the TOXSWA executable ('.exe') and TOXSWA template input file, needed in input folder ('SedDisFiles').
- Files specific to the TOXSWA application: FOCUS, GEM, DRAINBOW, also needed in input folder 'SedDisFiles\TOXSWA_inputs'.

Table 1 *Files required in the input folder 'SedDisFiles'.*

File Name	Description	File Extension	Source			
Files specific to the SedDis tool						
TOXSWA_SedDis.inp	SedDis Tool input file containing instructions to direct the tool.	.inp	The structure of this file is provided with this tool, but the file needs to be tailored to the model tested. Instructions in Section 5.4.1.			
fx.inp (x = 1, 2, 3)	Containing the relevant segmentations (require the same name as given in the TOXSWA_SedDis.inp file.	.inp	Files are provided in this tool. Provided the user would like to test the segmentation further, the creation of new files is required. Instructions in Paragraph 5.4.3.			
Files common for all TOXSWA simulations						
Ref.txw	TOXSWA template input file.	.txw	This file must be created by the user for the specific simulation to be tested. Instructions in Section 5.4.2.			
Meteostation.met	Meteorological data (file to copy in folder TOXSWA_inputs).	.met	Provided by the user			
Toxswa_xxxx.exe	TOXSWA Executable.	.exe	Provided by the user			
Scenario-specific files (source: provided by the user) **(These files must be copied in the folder SedDisFile\TOXSWA_inputs)**				**FOCUS**	**DRAINBOW**	**GEM**
File name	**Description**	**File extension**				
WestLand_C.s2t	GEM Hydrology	.s2t				x
Gem1.g2t	GEM Substance Output	.g2t				x
drainbow_1.e2t	PEARL drainage flow and substance output	.e2t			x	
fruitditch_2020.hyd	DRAINBOW hydrology	.hyd			x	
Herwijnen.meth	DRAINBOW hourly meteorology	.meth	Instead of Meteostation.met		x	
RunID-C1.p2t	FOCUS PRZM runoff flow and substance output	.p2t		x		
macroRunID_p.m2t	FOCUS MACRO drainage flow and substance output	.m2t		x		

Firstly, SedDis creates the inputs for the TOXSWA model, which are the TOXSWA template input files (.txw) tailored for each segmentation (and for the provided K_{om} value) and labelled according to the segmentation refinement (fx.txw). Then SedDis runs TOXSWA, creating the output files common for TOXSWA applications: notably the resulting summary file (RunID.sum), the detailed output file (RunID.out), and the log file (RunId.log). These files created by TOXSWA are described in the TOXSWA User guide (Beltman et al. (2018)).

5.3.2 Output files

The output files are:

1. The completed input file for the TOXSWA simulation:
   fx.txw — TOXSWA input file for each sediment segmentation, labelled according to the segmentation refinement.
2. The output of the TOXSWA simulation:
   fx.sum, fx.out, fx.log — The regular outputs files from the TOXSWA software are also created as the SedDis tool runs TOXSWA. Those files are named after the discretisation (fx, therefore f1, f2 etc).
3. A .csv file containing the results of the simulation:
   PECValues.csv — Csv file containing PEC values for each sediment segmentation for each K_{om} value.

5.4 Description of the SedDis input files

5.4.1 SedDis tool input file: TOXSWA_SedDis.inp

The SedDis tool first scans the input file (TOXSWA_SedDis.inp) to obtain the following information:

- Name of the executable.
- List of segmentations names ("table Discretisations").
- List of K_{om} values ("table Kom").

Note that the table may contain a single K_{om} value: the K_{om} value of the tested pesticide. For research purpose, the possibility to run the simulations for testing a range of K_{om} values is maintained. In this case, for each K_{om} in the K_{om} list, the module would create a new folder in the TOXSWA run folder.

Example 'TOXSWA_SedDis.inp' *File*[4]

```
*-----------------------------------------------

* Settings
*-----------------------------------------------
TOXSWA_33_03Oct2019.exe       Name of TOXSWA executable

table Discretisations
f1
f2
f3
f1std
f2std
f3std
end_table

table Kom
10000
end_table
```

5.4.2 TOXSWA Template file: ref.txw

The TOXSWA template input file ('ref.txw') is a copy of the TOXSWA template input file with the sediment profile omitted. An example is provided within the present tool (in the folder 'SedDis_tool_example_1'). The user will have to create a TOXSWA template input file ('.txw') tailored to the scenario the user wishes to test using the indications given in Section 6.3.

[4] The names of the files containing the discretisation should contain only letters and numbers for the code to function (no non-alphanumeric symbols such as "_"shall be employed).

5.4.3 Segment thickness files: fx.inp (f1.inp...)

The files containing the segmentations are named fx.inp (i.e. f1.inp, f2.inp….). The module will read the 'table Discretisations' and search for the corresponding segmentation files ('fx.inp') in the input folder. The contents of the segmentation input file is then inserted into a copy of the template file ('ref.txw'), renamed with corresponding segmentation label, where the line '<Sediment Profile>' is found.

In the FOCUS scenario, pesticides can be transported with runoff. It is then necessary to make sure that the sediment layer that receives the eroded sediment from runoff is of the same thickness than the top layer in the sediment discretisation table. This parameter is addressed in 'Section 8: Loadings' of the TOXSWA input file ('.txw') and is called ThiLayErs. The corresponding line should be copied and pasted to the segmentation file ('fx.inp') files and the value adjusted.

The segmentation file ('fx.inp') should also contain the sediment properties with the definition of the sediment profile.

Therefore, the files describing the segmentation contain:

- The desired segments thicknesses (as presented in the TOXSWA template input file (.txw) in Section 4: *SedimentProfile table: thickness and number of segments in horizon). See further information about the segments thicknesses in section A4.2. Avoid blank lines in the definition of the table. Further information concerning segments thicknesses in TOXSWA are available in Annex 1.
- The description of the properties of each horizon (as presented in the TOXSWA template input file (.txw) in Section 4: * SedimentProperties table: properties for each horizon). Those values must correspond to the simulation case; the values provided in the example therefore need to be adapted. Be aware that the number of horizons must be similar to the number of horizons in the preceding table (SedimentProfile). Avoid blank lines in the definition of the table.
- In the case of a FOCUS scenario, the definition of the thickness of the upper layer receiving the eroded sediment from runoff (ThiLayErs (m), in 'Section 8: Loadings'). Ideally, this value should be the same for all simulations: fine and standard.

Example segmentation file (f1.inp: fine segmentation)

```
* Table SedimentProfile
* ThiHor = thickness of horizon []
* NumLay = number of layers in horizon [1,]
table SedimentProfile
ThiHor NumLay
(m)
0.00024   8
0.00012   2
0.00024   2
0.0009    3
0.0015    2
0.004     2
0.003     1
0.01      2
0.03      3
0.02      1
0.03      1
end_table

Input      OptSedProperties ! Option sediment properties [Input, Calc]

* table specifying SedimentProperties for each horizon:
* Nr        = number horizon []
* Rho       =  bulk density [100 – 2000]
* CntOm     = organic matter mass content [0.0 – 1.0]
* ThetaSat  = saturated water content [0.1 – 0.95]
```

```
* CofDifRel = relative diffusion coefficient [0.0 – 1.0]
table  horizon SedimentProperties
Nr         Rho        CntOm      ThetaSat   CofDifRel
           (kg.m-3)   (kg.kg-1)  (m3.m-3)   (-)
1          800.       0.09       0.6        0.6
2          800.       0.09       0.6        0.6
3          800.       0.09       0.6        0.6
4          800.       0.09       0.6        0.6
5          800.       0.09       0.6        0.6
6          800.       0.09       0.6        0.6
7          800.       0.09       0.6        0.6
8          800.       0.09       0.6        0.6
9          800.       0.09       0.6        0.6
10         800.       0.09       0.6        0.6
11         800.       0.09       0.6        0.6
end_table

* Only for focus scenario : correction of the ThiLayErs
                           ! for output of (averaged) content [1e-5|1]
0.00024        ThiLayErs (m)       ! Thickness of upper sediment layer to which erosion
    mass
                                    ! is added [1e-5|1]
```

6 Running the tool

6.1 Example: Greenhouse scenario

6.1.1 Scenario, crop, application scheme, and properties of substance

This case study was performed for the greenhouse soilless scenario (Van der Linden, 2015; Wipfler, et al., 2015). A plant protection product was applied in a crop in a greenhouse grown on substrate in which the nutrient solution was recirculated. Recirculation water is released to surface water when the salinity of the recirculation water has become too high. The discharged recirculation water may still contain residues of the applied plant protection product. The substance enter the ditch at the upstream boundary of the ditch.

The output of SEM for example substance EXGE1 was used, with a single application to the nutrient solution in the greenhouse on 15 April at 2 AM at 0.84 kg for roses. Substance properties of EXGE1 are given in Annex 2, Table A1. The sorption coefficient for organic matter in suspended solids was set to zero.

6.1.2 Running the example

After installing the tool (see Chapter 4), the example can be run as follows:

1. Open the command prompt and run the command line "python SedDis_Tool.py".
2. Follow the instructions from the different message boxes. The first message box requires you to select the input file (TOXSWA_SedDis.inp) provided with the tool (3). Once chosen, you hit "exit message box".
3. You will then need to provide the number of cores you want to use for running TOXSWA (Figure 4), we advise to select as many cores as simulations, hence here 6, and proceed. Then you will be offered to run TOXSWA (Figure 5) and hit the "yes" button.
4. Command windows will open, each of them running a simulation. Let the simulations run until completion. Normally, one simulation ends without warnings or errors, and the command windows will close itself. At the start of the simulation, error ('.ERR') and warning files are created. When both files are removed and replaced by a file "toxswa.ok", this indicates that the run has been finalized successfully. TOXSWA will create an output of the simulation (fx.sum).
5. Once the simulation is completed, a new window open to select the destination of the output file (Figure 6). It is possible to select another folder than the advised SedDis folder if the user wants to store the output in another directory.
   The tool extracts the PECsw values from the output files for the different simulations and stores them as a table in a CSV file (PECvalue.csv) located in the folder containing the results (SedDis folder). The values in the CSV file should be copied and paste manually to the Excel file (SedDis_Output_Interpretation.xlsx) provided with the tool. The results can then be visualised and printed or converted to a PDF file (presented in the next section).

For information, running the example takes 25 minutes, using 6 cores on an Intel(R) Xeon(R) W-2235 CPU @ 3.80GHz 3.79 GHz computer.

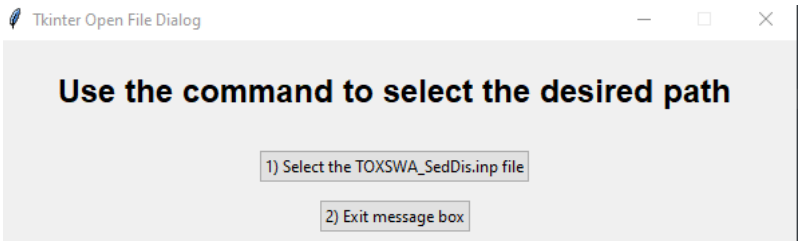

Figure 3 *Select the path through selecting the input file.*

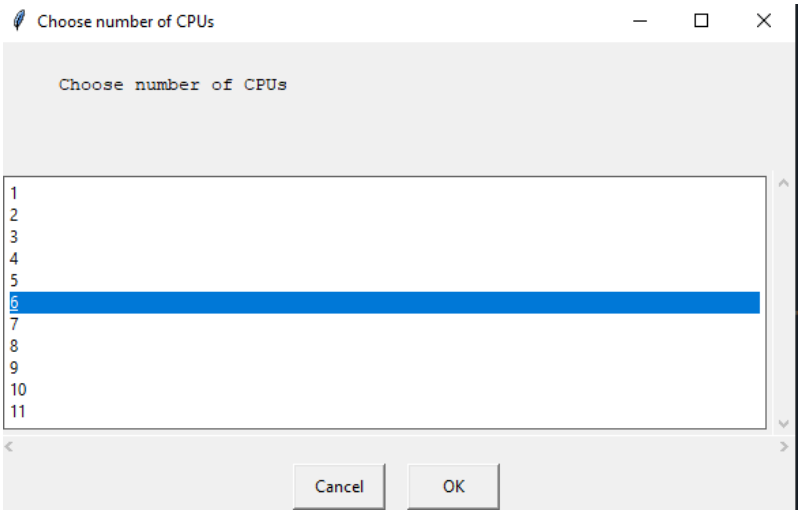

Figure 4 *Select the number of CPUs.*

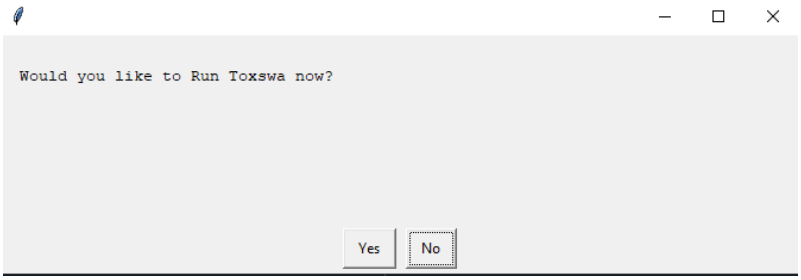

Figure 5 *Run TOXSWA.*

Figure 6 *Select the output folder (SedDis folder is recommended).*

6.2 Presenting and interpreting the results

Once the simulation is finished, the data are printed to a CSV file. Once copied and pasted manually in the dedicated cells to the Excel file for visualisation and interpretation of results ('Results_simulation.xlsx'), the results are presented as follows (Figures 7 to 9). A detailed interpretation is provided in Annex 3. The example provided is based on the case study described in Chapter 6, which uses the greenhouse soilless scenario. While the case study presented in Annex 3 was performed for a large range of K_{om} values, the example below simulates one unique value of K_{om} to illustrate the case of a fine segmentation to standard segmentation comparison for a given pesticide.

Author or repport number
Date

Testing segments thicknesses of the sediment layer in TOXSWA from the SedDis (sediment discretization) tool

SedDis tool v.1

Insert here any comment

Simulations names

Insert the name of your simulation

	Fine segmentation		Standard segmentation

Sorption coefficient

Insert the Kom value of the tested chemical

Kom (L/kg)	1000.00		1000.00

Simulation results (here PEC value µg/L)

Insert the results from the simulation

f1	537	**f1std**	539.7
f2	539.6	**f2std**	554.7
f3	550.9	**f3std**	588.7

Acceptable error range

Insert the acceptable error range

Error	2%

Figure 7a The results from the simulations and additional information can be given in the grey areas (simulation names, author of the report).

The results below are automatic calculations, changing the content of the cells is not permitted.

Segmentation refinement ratio (or indicator)

Ratio between the larger segmentation and the thinner segmentation - here the same ratio has to be picked between f3 and f2 and f2 and f1.

r	2		2

Normalized segmentation

The grid size relative to the most refined one

	0		0
f1	1	f1std	1
f2	2	f2std	2
f3	4	f3std	4

Order of convergence (case of 3 segmentation refinement steps)

$$p = \frac{\ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right)}{\ln(r)}$$

p	2.120	1.181

Relative error for f1

$$\varepsilon_{21} = \frac{f_2 - f_1}{f_1}$$

ε21	0.005	0.028

Continuum value for zero

The continuum value is the value for the segmentation going to infinitely small.

$$f_{h=0} \cong f_2 + \frac{(f_1 - f_2)r^p}{r^p - 1}$$

f(h=0)	536.2	527.9

Factor of safety

The factor of safety is recommended to be Fs = 3.0 for comparisons of two segmentations and Fs = 1.25 for comparisons over three or more segmentations (this case).

Fs	1.25	1.25

Fractionnal error as fx/f(h=0)		
A0	1	1
A1	1.001	1.022
A2	1.006	1.051
A3	1.027	1.115

Fractionnal error as a percentage of f(h=0)		
A1	0.14%	2.24%
A2	0.63%	5.09%
A3	2.74%	11.53%

Grid convergence index

The GCI is a measure of the percentage the computed value is away from the value of the asymptotic numerical value.

$$GCI_{21} = \frac{F_s|\varepsilon_{21}|}{r_{21}^p - 1}$$

For the finest segmentation (f1):

CGI21	0.18%	2.74%

Figure 7b *The different parameters relevant for the interpretation are then calculated. The cells with calculations are protected and cannot be modified.*

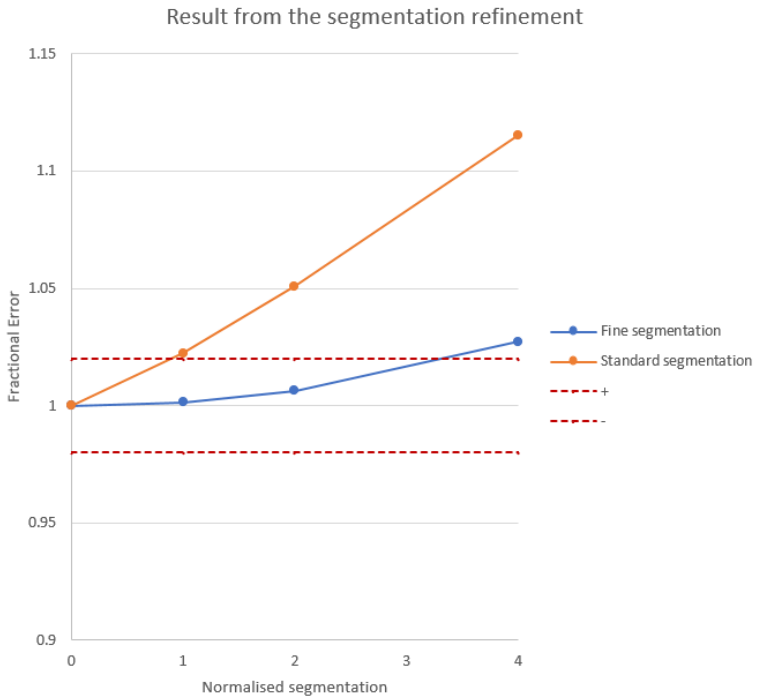

Figure 8 *Output figure: Figure 1 PEC calculated for the different segmentations divided by continuum value PEC as function of normalized segmentations for standard- and fine segmentations.*

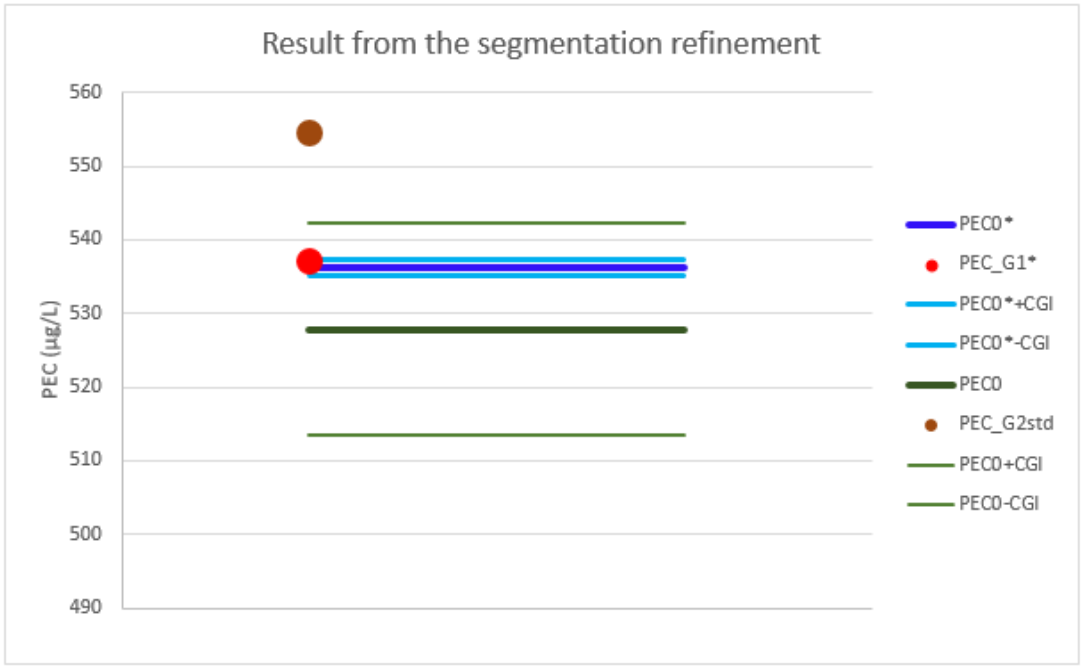

Fig 2. PEC-$f^*_{h=0}$ (thick blue line), PEC-$f_{h=0}$ (thick dark green line), PEC-$f^*_{h=0}$ ± CGI (blue lines), PEC-fh=0 ± CGI (thin green lines), PEC-f_1* (red circle) and PEC-f_2 (brown circle) for K_{om} 1000 L/kg

Figure 9 *Output figure: Figure 2 PEC-f*h=0 (thick blue line), PEC-fh=0 (thick dark green line), PEC-f*h=0 ± CGI (thin blue lines), PEC-fh=0 ± CGI (thin green lines), PEC-f1* (red circle) and PEC-f2 (brown circle) for Kom 1000 L/kg.*

6.3 Running with your own data

This is the instruction for when SedDis is used for one specific K_{om} value.

This tool is meant to be used in combination with input data generated by a risk assessment application that includes TOXSWA and was tested for GEM and DRAINBOW. We assume that the user ran a simulation and, therefore, created the required input files.

1. Create the following path: Simulation /SedDisFiles/TOXSWA_Inputs. The term "Simulation" in this path is an example and can be modified, whilst the file names 'SedDisFiles' and 'TOXSWA_Inputs' cannot be modified.
2. To directory TOXSWA_Inputs, copy the meteorological data (.met) file corresponding to your simulation as well as the scenario-specific files listed in Table 1 (for example: .s2t).
3. Create the TOXSWA_SedDis.inp file following the instructions in Section 5.4.1. The K_{om} value of the pesticide is to be provided in the Table of K_{om} values (table Kom)[5].
4. To directory SedDisFiles, copy the following files:
   a. the discretisation files (f1.inp to f3.inp and f1std.inp to f3std.inp, examples of those files are provided with the SedDis tool, but the sediment properties have to be adapted to the specific simulation using the values in the TOXSWA input file ('.txw').
   b. the executable (e.g. toxswa_focus_3.exe – verify that the file name indicated in the SedDis input file (TOXSWA_SedDis.inp) corresponds to the executable).
   c. the TOXSWA template input .txw for your simulation has to be renamed to 'ref.txw'.
   d. the TOXSWA_SedDis.inp file (created at step 3).
5. Open the TOXSWA template input file ('ref.txw') and implement the following modifications:
   a. In Section 4, the sediment profile and the sediment properties blocks must be replaced with the text <Sediment Profile>.
   b. In Section 1, Section 5, Section 8: file paths are provided. It is recommended to adjust the path information, as in the following examples, for the software to use the appropriate path:
      i. Section 1: D:\SWASH\TOXSWA\data => D:\data
      ii. Section 5: D:\SWASH\PRZM\MET\R1NOIRR.MET => R1NOIRR.MET
      iii. Section 8: D:\SWASHprojects\project_EXSW2_2020\PRZM\cereals_winter\00010-C1.p2t => 00010-C1.p2t (example for a scenario-specific file)
   c. *(optional – only for research) In Section 7b, replace the Sorption coefficient in the sediment (KomSed_molecule) with the text <Kom>.*
   d. *(optional: FOCUS scenarios) In the case of FOCUS simulations, as the value for ThiLayErs must be modified, it is recommended to remove the line containing the information relative to the thickness of the layer receiving the eroded sediment (ThiLayErs parameter) from the TOXSWA template input file ('ref.txw') file. The value provided in the discretisation file ('fx.inp') will be copied to the TOXSWA template input file ('.txw')[6].*

Now that the input files are prepared:

6. Open the command prompt and run "python SedDis_Tool.py".
7. Follow the instruction of the different message boxes.
   a. For the first message box, you need to select the SedDis input file (TOXSWA_SedDis.inp).
   b. The number of CPUs: We recommend matching the number of simulations (in most cases: six (6)) or the maximum numbers of CPU in the list.
   c. For the third message box, you need to select the output folder (SedDis).
8. Let the simulation run until completion.

The data are printed to an output file ('PECvalue.csv') in the folder containing the results (SedDis folder). The values in the output file have to be manually copied and paste into the Excel tool ("SedDis_Output_Interpretation.xlsx") provided. The results can be printed as a PDF file.

[5] Note that the user can skip the step 5.c., in which case the K_{om} value indicated in the Table of K_{om} will not be used in the simulation; however, a numerical value has to be indicated in the Table of K_{om} to avoid error when running the SedDis tool.

[6] If, by accident, two records containing ThiLayErs are given in the TOXSWA input file, the simulation will use value given in the first record.

6.4 Incomplete TOXSWA runs

No value will be printed in the output file ('PECvalue.csv') for incomplete runs. The reason for failure can be investigated by the user:

Completion of the runs
At the start of TOXSWA runs, a file reporting the log of the error ('.ERR') is created in the folder containing the simulation input files and results (for instance, 'SedDis/1000/f1'). If the run is not completed, the error log remains. The error log will contain the reason for failing. Note that when TOXSWA ran with the SedDis tool, the error log might be empty. The run for which this occurs can be started manually. For instance, by double clicking the corresponding batch file ('.bat') in the simulation folder.

Time step error
The simulation may have stopped due to a time step error, as indicated in the error log ('.ERR'). Then, also a recommendation for an appropriate maximal time step is provided. This value can be adjusted manually in the TOXSWA template input file ('.txw') file in Section 1 (parameter MaxTimStpWat or MaxTimStpSed, based on the recommendation in the error log). After saving the modification, the run must be launched again (double-click on the batch file ('.bat')). The result data will need to be collected manually from the result file ('.sum') at the line indicating the 50-percentile peak concentration (example: '* The 50-percentile peak concentration of EXGE1 is 550.9 ug/L').

References

Adriaanse, P.I. 1996. *Fate of pesticides in field ditches: The TOXSWA simulation model.* Wageningen: DLO Winand Staring Center for Integrated Land, Soil and Water Research (SC-DLO), 1996.

Beltman, W.H.J., M.M.S. ter Horst, P.I. Adriaanse & A. de Jong. 2018. *WOt-technical report 126. Manual for FCOUS_TOXSWA v5.5.3 and for expert use of TOXSWA kernel v3.3.* Wageningen: Satutory Reasearch Tasks Unite for Nature & the Environment, 2018.

Van der Linden, A.M.A., E.A. van Os, E.L. Wipfler, A.A. Cornelese, D.J.W. Ludeking, T. Vermeulen. 2015. *Scenarios for exposure of aquatic organisms to plant protection products in the Netherlands. Soilless cultivations in greenhouses*: RIVM report 2015-012, 2015.

Wipfler, E.L., C. Vink, M.M.S. ter Horst & A. de Jong. 2015. *Manual GEM 1.1.1, Greenhouse Emission Model, exposure assessment tool for Plant Protection Products used in greenhouse crop cultivation.* Wageningen: Alterra report 2614, 2015.

Justification

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The report has been reviewed and approved by Dr. S. Boersma (WUR-Biometris).

This study was supervised by Erwin van Boekel (Wot N&M, theme Agri-environment*)] and Eelco Riemens (Ministry of Agriculture, Nature and Food Quality). The research methods and research approach were supervised by members of ERA (Team Environmental Risk Assessment, WENR).*

Approved by External contact person

position: policy officer

name: Eelco Riemens

date: 9-1-2023

Approved by Internal contact person

name: Erwin van Boekel

date: 20-12-2022

Annex 1 Sediment segmentations used in scenarios

For FOCUS (2002), two sediment segmentations were defined. The fine sediment segment thickness is given in Figure A1, and the standard segmentation is given in Figure A2.

```
*-------------------------------------------------------------------------------
* Section 4: Sediment section
*-------------------------------------------------------------------------------

Benschop      SedimentTypeID ! Name of sediment type


* Table SedimentProfile
* ThiHor = thickness of horizon []
* NumSeg = number of segments in horizon [1,]
table SedimentProfile
ThiHor NumSeg
(m)
0.00024   8
0.00012   2
0.00024   2
0.0009    3
0.0015    2
0.004     2
0.003     1
0.01      2
0.03      3
0.02      1
0.03      1
end_table

Input      OptSedProperties ! Option sediment properties [Input, Calc]

* table specifying SedimentProperties for each horizon:
* Nr         = number horizon []
* Rho        =  bulk density [100|2000]
* CntOm      = organic matter mass content [0.0|1.0]
* ThetaSat   = saturated water content [0.1|0.95]
* CofDifRel = relative diffusion coefficient [0.0|1.0]
table  horizon SedimentProperties
Nr      Rho         CntOm      ThetaSat    CofDifRel
        (kg.m-3)    (kg.kg-1)  (m3.m-3)    (-)
1       800         0.09       0.68        0.56
2       800         0.09       0.68        0.56
3       800         0.09       0.68        0.56
4       800         0.09       0.68        0.56
5       800         0.09       0.68        0.56
6       800         0.09       0.68        0.56
7       800         0.09       0.68        0.56
8       800         0.09       0.68        0.56
9       800         0.09       0.68        0.56
10      800         0.09       0.68        0.56
11      800         0.09       0.68        0.56
end_table
```

Figure A1 *Section 4 from the TOXSWA template input file (*.txw) showing the fine sediment segmentation and properties for the horizons.*

```
*-------------------------------------------------------------------------------
* Section 4: Sediment section
*-------------------------------------------------------------------------------

Benschop      SedimentTypeID ! Name of sediment type


* Table SedimentProfile
* ThiHor = thickness of horizon []
* NumSeg = number of segments in horizon [1,]
table SedimentProfile
ThiHor NumSeg
(m)
0.004    4
0.006    3
0.01     2
0.03     3
0.02     1
0.09     3
end_table

Input      OptSedProperties ! Option sediment properties [Input, Calc]

* table specifying SedimentProperties for each horizon:
* Nr        = number horizon []
* Rho       =  bulk density [100|2000]
* CntOm     = organic matter mass content [0.0|1.0]
* ThetaSat  = saturated water content [0.1|0.95]
* CofDifRel = relative diffusion coefficient [0.0|1.0]
table  horizon SedimentProperties
Nr     Rho         CntOm     ThetaSat   CofDifRel
       (kg.m-3)    (kg.kg-1)  (m3.m-3)   (-)
1      800         0.09       0.68       0.56
2      800         0.09       0.68       0.56
3      800         0.09       0.68       0.56
4      800         0.09       0.68       0.56
5      800         0.09       0.68       0.56
6      800         0.09       0.68       0.56
end_table
```

Figure A2 *Section 4 from the TOXSWA template input file (*.txw) showing the standard sediment segmentation and properties for the horizons.*

Annex 2 Substance properties and application scheme

In Table A1, the input values for the GEM soilless calculation are given.

Table A1 *Values of substance properties and applications used in the GEM soil-less calculation.*

Property	Units	Value
Molar mass	$g.mol^{-1}$	300
Saturated vapour pressure	Pa	$1 \cdot 10^{-10}$
Reference temperature for saturated vapour pressure	°C	20
Molar enthalpy of the vaporisation process	kJ/mol	95
Solubility	mg/L	100
Reference temperature for water solubility	°C	20
Molar enthalpy of the dissolution	kJ/mol	27
Diffusion		
diffusion coefficient	$m^2.d^{-1}$	$4.3 \cdot 10^{-5}$
Transformation in water		
Half-life in water (lumped)	d	1000
Temperature at which half-life in water was measured	°C	20
Molar activation enthalpy of transformation	kJ/mol	75
Transformation in sediment		
Half-life transformation in sediment	d	1000
Temperature at which half-life in sediment was measured	°C	20
Molar activation enthalpy of transformation in sediment	kJ/mol	65.4
Sorption to sediment		
Coefficient of equilibrium sorption in sediment	L/kg	0
Reference concentration in liquid phase in sediment	mg/L	1
Freundlich exponent in sediment	-	0.9
Sorption to suspended solids		
Concentration suspended solids	g/m^3	15
Coefficient of equilibrium sorption of suspended solids	L/kg	0
Reference concentration	mg/L	1
Freundlich exponent	-	0.9
Sorption to macrophytes		
Coefficient for linear sorption on macrophytes	(L/kg)	0

Annex 3 Case study

A3.1 Scenario, crop, application scheme, and properties of substance

This case study was performed done for the greenhouse soil-less scenario (Van der Linden, 2015; Wipfler, et al., 2015). A plant protection product is applied in a crop in a greenhouse grown on substrate in which the nutrient solution was recirculated. Recirculation water is released to surface water when the salinity of the recirculation water has become too high. The discharged recirculation water may still contain residues of the applied plant protection product. The substance enters the ditch at the upstream boundary of the ditch.

Output of the Substance Emission Model (SEM) is used for the entry of substance at the upstream boundary of the ditch. SEM was run with a single application of example substance, EXGE1, to the nutrient solution in the greenhouse on 15 April at 2 AM at 0.84 kg for roses. Substance properties are given of EXGE1 in Annex 2, Table A1. For the sorption coefficient for organic matter in sediment, the value varied as given in Section A3.3. The sorption coefficient for organic matter in suspended solids was set to zero.

A3.2 Segmentation of the sediment layer

The two sediment segmentation currently used in TOXSWA are a fine segmentation and a standard sediment segmentation. Both are given in Annex 1. In the following, these segmentations (or grid) will be referred to as fine (G_{fine}) and standard (G_{std}).

The convergence of one of the segmentations (fine or standard) is obtained by running simulations with a series of three segmentations with incremental discretisation, i.e. with incremental segments thicknesses. In the following, we use the notations G_1*, G_2* and G_3* for the three segmentations derived from the fine segmentation, with G_1* being similar to G_{fine}. The notations G_1, G_2 and G_3 are used for the three segmentations derived from the standard segmentation, with G_2 being G_{std}.

The finest segmentation corresponds to the first levels, G_1* and G_1. From this fine segmentation, two levels of coarser segmentations, respectively G_2* and G_3*, and G_2 and G_3, are made by combining the thickness of two segments in each consecutive step. The normalized segmentation is defined as the segments thickness ratio (r) relative to the segment thickness of most refined segmentation, hence, here the normalized segmentation for G_2*/G_2 is 2 and for G_3*/G_3 is 4.

For G_1*, one segment was added to the total number of segments of G_{fine} to enable the division by 4. This segment was added at the bottom of the sediment layer. For G_2 a similar procedure was followed[7]. The segmentations are given in Table A2 and Table A3, respectively. The depth indicates the depth of the node in the centre of the segment.

[7] For segmentations derived from the standard segmentation, the standard segmentation is not derived from G_1, but from G_2. A series of segmentation based on G_1 resulted in a G_3 segmentation being too coarse. Allocating the standard segmentation to G_1 with its derived segmentations G_2 (= G_3 in Table A2b) and G_3 (= 1x0.004, 1x0.0875, 1x0.03575, 1x0.1055 m) led to inconsistent results. The difference in PECs between then G_2 and G_3 were smaller than the difference in PECs between the G_1 and G_2 segmentations, resulting in negative p values (as explained in this Section), giving continuum value $f_{h=0}$ PECs (see also this section) higher than G_3 PECs. Hence, this series allocating TOXSWA's standard segmentation to G_1 could not be used. TOXSWA's standard segmentation was allocated to G_2, and G_1 and G_3 segmentations were derived from this G_2 segmentation.

Table A2a *Segments thicknesses of the fine segmentation (= G_1*); thicknesses entered in TOXSWA input file.*

G_1*	Thickness (m)	Depth (m)	G_2*	Thickness (m)	Depth (m)	G_3*	Thickness (m)	Depth (m)
1	0.00003	0.000015	1	0.00006	0.00003	1	0.00012	0.00006
2	0.00003	0.000045						
3	0.00003	0.000075	2	0.00006	0.00009			
4	0.00003	0.000105						
5	0.00003	0.000135	3	0.00006	0.00015	2	0.00012	0.00018
6	0.00003	0.000165						
7	0.00003	0.000195	4	0.00006	0.00021			
8	0.00003	0.000225						
9	0.00006	0.00027	5	0.00012	0.0003	3	0.0003	0.00039
10	0.00006	0.00033						
11	0.00012	0.00042	6	0.00024	0.00048			
12	0.00012	0.00054						
13	0.0003	0.00075	7	0.0006	0.0009	4	0.0014325	0.00125625
14	0.0003	0.00105						
15	0.0003	0.00135	8	0.000825	0.001613			
16	0.00075	0.001875						
17	0.00075	0.002625	9	0.002575	0.003313	5	0.0066175	0.00528125
18	0.002	0.004						
19	0.002	0.006	10	0.0053	0.00725			
20	0.003	0.0085						
21	0.005	0.0125	11	0.0102	0.015	6	0.02782	0.0225
22	0.005	0.0175						
23	0.01	0.025	12	0.0198	0.03			
24	0.01	0.035						
25	0.01	0.045	13	0.0252	0.0525	7	0.07968	0.07625
26	0.02	0.06						
27	0.03	0.085	14	0.0698	0.1			
28	0.03	0.115						
total	0.13			0.1349			0.11609	

Table A2b *Segments thicknesses of the standard segmentation(= G_2); thicknesses entered in the TOXSWA input file.*

G_1	Thickness (m)	Depth (m)	G_2	Thickness (m)	Depth (m)	G_3	Thickness (m)	Depth (m)
1	0.0005	0.00025	1	0.001	0.0005	1	0.002	0.001
2	0.0005	0.00075						
3	0.0005	0.00125	2	0.001	0.0015			
4	0.0005	0.00175						
5	0.0005	0.00225	3	0.001	0.0025	2	0.002	0.003
6	0.0005	0.00275						
7	0.0005	0.00325	4	0.001	0.0035			
8	0.0005	0.00375						
9	0.001	0.0045	5	0.002	0.005	3	0.004	0.006
10	0.001	0.0055						
11	0.001	0.0065	6	0.002	0.007			
12	0.001	0.0075						
13	0.001	0.0085	7	0.002	0.009	4	0.0055	0.01075
14	0.001	0.0095						
15	0.0025	0.01125	8	0.005	0.0125			
16	0.0025	0.01375						
17	0.0025	0.01625	9	0.005	0.0175	5	0.0155	0.02125
18	0.0025	0.01875						
19	0.005	0.0225	10	0.01	0.025			
20	0.005	0.0275						
21	0.005	0.0325	11	0.01	0.035	6	0.022	0.04
22	0.005	0.0375						
23	0.005	0.0425	12	0.01	0.045			
24	0.005	0.0475						
25	0.01	0.055	13	0.02	0.06	7	0.043	0.0725
26	0.01	0.065						
27	0.015	0.0775	14	0.03	0.085			
28	0.015	0.0925						
29	0.015	0.1075	15	0.03	0.115	8	0.072	0.13
30	0.015	0.1225						
31	0.015	0.1375	16	0.03	0.145			
32	0.015	0.1525						
total	0.16			0.16			0.16	

The segmentation files used in the example are provided in the SedDis tool under the names: f1, f2 and f3 for the fine segmentations and f1std, f2std and f3std for the standard segmentation.

If the reader wants to test a finer segmentation, it is necessary to follow a similar strategy as above. It is recommended to keep the finest discretisation in the discretisation file ('f1.inp') and to increment the discretisation with the same ratio between f1 and f2 than f2 and f3 to be able to use the tool. Using different ratios between the segmentations is possible but requires adaptation of the calculations as compared to that provided in the tool.

The method makes use of the segmentation concept. The segmentation of the first level is the finest segmentation considered. From this fine segmentation, one can build the *n* levels of coarser segmentation s by dividing each layer into two in each consecutive step. The normalized segmentation is the segmentation size relative to the most refined one.

A3.3 Sorption coefficient values

In this study, the sorption coefficient (K_{om}) was varied in order to illustrate the results that can be expected for a large range of molecules. K_{om} range used is 1, 10, 100, 1 000, 10 000, 100 000 and 1 000 000 L/kg, as per those used by Adriaanse et al. (2015) in its Annex 12.1.

A3.4 Predicted Environmental Concentrations

The TOXSWA model was run for the test case using the K_{om} range, as given in Section A3.3, and with segmentations of the sediment layer, as given in Table A2. Runs with the fine sediment segmentation for K_{om} 1, 100 and 1000 L/kg did not converge, and using smaller time steps for the simulation did not solve this. The combination of a low sorption coefficient with a fine segmentation cannot be solved with the numerical solution applied by TOXSWA. For some runs (G_1; 1000 L/kg), the maximal time step for sediment was decreased from 600 s (the default time step) to 100 s, because negative concentrations were calculated when using larger time steps.

In Table A3, the PECs are shown, these are indicated by f_x, with x being the segmentation refinement indicator, and f_1 is the resulting PEC for segmentation G_1 and f_1* for segmentation G_1*, etc.

Table A3 *Predicted Environmental Concentrations calculated with greenhouse soil-less scenario with segmentations as given in Table 1 (fine) and 2 (standard). PECs are given for a range of Kom values of the example substance (F= failed run). The columns in bold indicate the segmentations used in GEM.*

K_{om} (L/kg)	Fine			Standard		
	f_1* (µg/L)	**f_2*** (µg/L)	**f_3*** (µg/L)	**f_1** (µg/L)	**f_2** (µg/L)	**f_3** (µg/L)
1	**F**	F	F	698.4	**698.7**	699.1
10	**F**	F	F	690	**690.2**	690.8
100	**F**	651.4	657.4	649.7	**650.3**	652.6
1 000	**537**	539.6	550.9	539.7	**554.7**	588.7
10 000	**373.6**	377	388	458	**528.9**	584.3
100 000	**206.6**	227.9	264.5	420.8	**601.8**	772
1 000 000	**115.1**	152.6	209.6	416.4	**598.3**	770.6

PECs increase going from the finest (f_1 and f_1*) to the coarsest segmentation (f_3 and f_3*) for all combinations of segmentations and sorption coefficients. The year corresponding to the 50-pecentile may differ per K_{om} and per segmentation.

For consistency in the analysis, we used the 50th percentile year of the finest segmentation, i.e. G1 and G1*, which was 2005. Combinations for which the 50th percentile year is not 2005 are: finest segmentation / K_{om} 1 000 000 L/kg (2002), standard segmentation/ K_{om} ≥ 100 000 L/kg (2002), and other K_{om} ≥ 1000 L/kg and converging runs (2004).

Continuum value, error and grid convergence index
Next, the continuum value $f_{h=0}$ was calculated with Equation 1. Also, the order of convergence p was calculated with Equation 2, the error e was calculated with Equation 4 and the CGI_{fine} with Eq. (5). The results are given in Table A4.

The continuum PEC values are always lower than the PEC value calculated with the finest segmentation. For both fine and standard spacings, the continuum PEC values decrease with increasing K_{om}, which is expected, as a larger part of the substance mass will sorb to the sediment organic matter.

The theoretical order of convergence based on the applied segmentation refinement is 2.0. In the table, for most triplets the calculated order of convergence, p, is lower than 2, except for the fine segmentation for K_{om} values 100-1000 L/kg, and for the standard segmentation for K_{om} above 10000 L/kg (included). For situations where p differs from 2, possible sources of error are due to grid stretching, segmentation quality, non-linearities in the solution, presence of shocks, turbulence modelling, and perhaps other factors. For the TOXSWA case, this might be due to the interaction between water and sediment. The concentration in the water layer above the sediment is a source and sink for the sediment via diffusion. The changes in concentration in the water are marked at hourly time scales, whereas this is much slower for the concentration diffusion in sediment. This is likely to lead to non-linearities in the solution.

For the standard segmentation and K_{om} > 1000 L/kg, the order of convergence p is less than 1, which means that the difference between the results obtained with the larger segmentations (f_2 and f_3) is smaller than for the smaller segmentations (f_1 and f_2). The larger segmentations (and notably the standard segmentation) should not be used for the highest K_{om} (above switch value of TOXSWA for GEM). Therefore, these results are ignored, and the continuum PEC value is not calculated, nor is the relative error and the CGI for these simulations.

The relative error is a simple estimate for how close the f_2 value is to f_1. So, e.g. for G_1/K_{om} 1 000 000 L/kg, e = 0.326; the f_2* value is 32.6% higher than the f_1* value. Note that the relative error should not be used as an error indicator because it does not take into account r or p (Wipfler et al., 2018, p.18).

The grid convergence index (*CGI*) was suggested as a consistent manner to report results, indicating an error band. Three segmentations are compared, hence, the factor of safety F_s = 1.25 (see Section 3.1). Using Equations 4 and 5, the value of *CGI* for comparison of two segmentations was calculated. Hence, for the example of fine/K_{om} 1 000 000 L/kg, *CGI* = 78.3%; an error band of 78.3%. For K_{om} of 100 000 L/kg the CGI was 17.9%. For the fine segmentation, the other K_{om} values had the error band (CGI) < 2%.

For the standard segmentation up to K_{om} 1000 L/kg *CGI* is =< 2%. For K_{om} of 10 000 L/kg CGI is superior to 2% and for higher K_{om} CGI was not calculated.

Table A4 *Continuum value for PEC (fh=0), order of convergence (p), error (e) and error band (≈ grid convergence index, CGIfine) derived from PEC from the greenhouse soil-less scenario with segmentations as given in Table 1 (fine) and 2 (standard) and for a range of Kom values of the substance in sediment. (F = failed run, N = not considered in the analysis).*

K_{om} (L/kg)	Fine				standard			
	$f_{h=0}$* (µg/L)	*P*	*e*	*CGI* (%)	$f_{h=0}$ (µg/L)	*p*	*e*	*CGI* (%)
1	F	F	F	F	697.5	0.415	0.0004	0.16%
10	F	F	F	F	689.9	1.585	0.0003	0.02%
100	F	F	F	F	649.5	1.939	0.0009	0.04%
1 000	536.2	2.120	0.0048	0.18%	527.9	1.181	0.0278	2.74%
10 000	372.1	1.694	0.0091	0.51%	N	-0.36	N	N
100 000	176.9	0.781	0.1031	17.94%	N	-0.09	N	N
1 000 000	43.0	0.604	0.3258	78.32%	N	-0.08	N	N

A3.5 Fractional error

We calculated the fractional error *A* for each of the *f*-values with Equation 3, using the continuum values from Table 4. Results are shown in Table 5.

The fractional error, which is the error made when using a specific segmentation compared to the $f_{h=0}$ situation, increases going from the finest (G_1 and G_1*) to the coarsest spacing (G_3 and G_3*), for all series of three. This is consistent with Table 3 and 4. Note that in Table A4 the parameters *e* and *CGI* are calculated without using $f_{h=0}$, whereas the fractional result in Table A5 is based on $f_{h=0}$.

The f_1* column in Table A5 shows that up to K_{om} 10 000 L/kg the fractional error for the fine segmentation is < 0.02, hence, the overestimation of the calculated concentration is less than a fraction of 0.02, i.e. less than 2%. For K_{om} 1 000 000 L/kg the overestimation of the concentration is 167%. In GEM the fine segmentation is used for K_{om} > 1000 L/kg. For K_{om} < 1000 L/kg *A* could not be calculated due to convergence problems.

The f_2 column in Table A5 shows that for the standard segmentation up to K_{om} 1 000 L/kg the fractional error is < 0.004, hence, the overestimation of the calculated concentration is less than 0.4%. For K_{om} > 1000 L/kg it was not possible to run the simulations. In GEM, the standard segmentation G_2 is used for K_{om} ≤ 1000 L/kg.

In Figures A3a and b, PEC calculated for the segmentation relative to the PEC value of $f_{h=0}$ (Table A5) are plotted against normalized segmentation. The dashed lines (= 1±0.02) indicate a fractional error *A* of 2%, considered the acceptable limit.

Figure A3a shows that for fine segmentation, using normalized segmentation 1 (=G_1*) or 2 (**=**G_2*) overestimates PEC more than 2% for K_{om} ≥ 100 000 L/kg. Using normalized segmentation 4 (**=**G_3*) overestimates PEC values more than 2% for all K_{om} for which simulations were converging.

For standard segmentation the error associated with the segments thicknesses is larger, i.e. using normalized segmentation 1 (=G_1), 2 (**=**G_2), or 4 (**=**G_3) overestimates PEC more than 2% for K_{om} 1 000 L/kg.

Table A5 *Fractional error (A) of PEC calculated with greenhouse soil-less scenario with three segmentations based on fine sediment segmentation (= G1*) and three segmentations based on standard segmentation (=G2). Fractional results are given for a range of Kom values of the substance in sediment. Combinations that have an error > 2% are marked in yellow. (F = failed run, N = not considered further in the analysis).*

K_{om} (L/kg)	fine			standard		
	A f_1* (-)	***A*** f_2* (-)	***A*** f_3* (-)	***A*** f_1 (-)	***A*** f_2 (-)	***A*** f_3 (-)
1	F	F	F	1.00129	1.00172	1.00229
10	F	F	F	1.00014	1.00043	1.00130
100	F	0.99079	0.99992	1.00033	1.00125	1.00479
1 000	1.00145	1.00630	1.02737	1.02243	1.05085	1.11526
10 000	1.00409	1.01323	1.04279	N	N	N
100 000	1.16758	1.28796	1.49480	N	N	N
1 000 000	2.67770	3.55011	4.87616	N	N	N

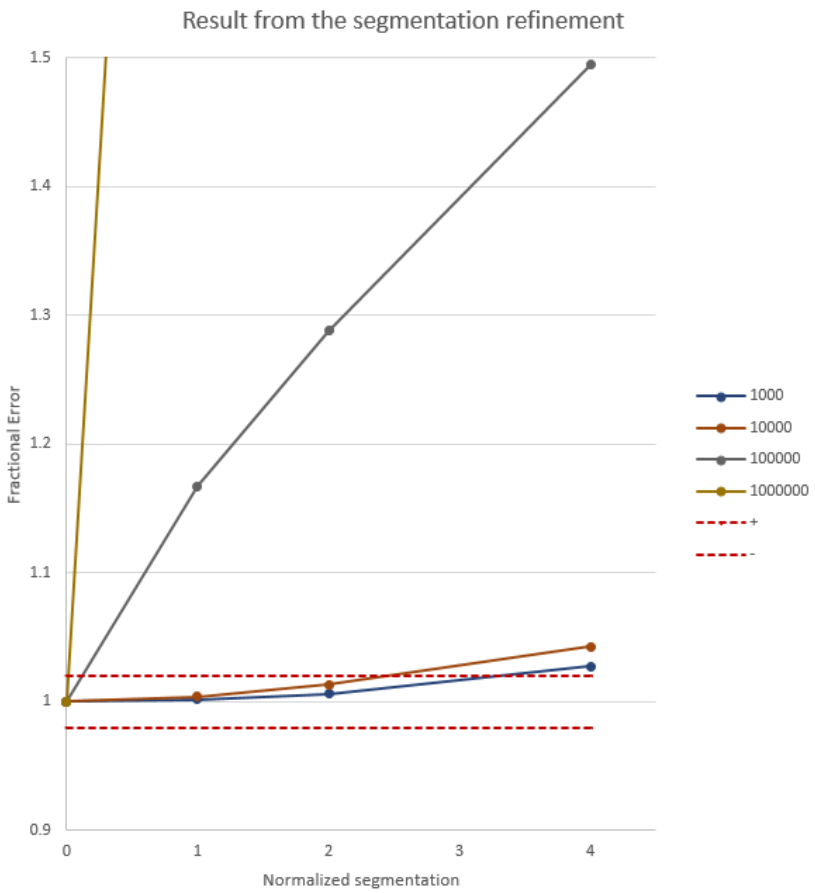

Figure A3a *PEC calculated for the different segmentations divided by continuum value for PEC as function of normalized segmentation for different values of Kom for fine segmentation.*

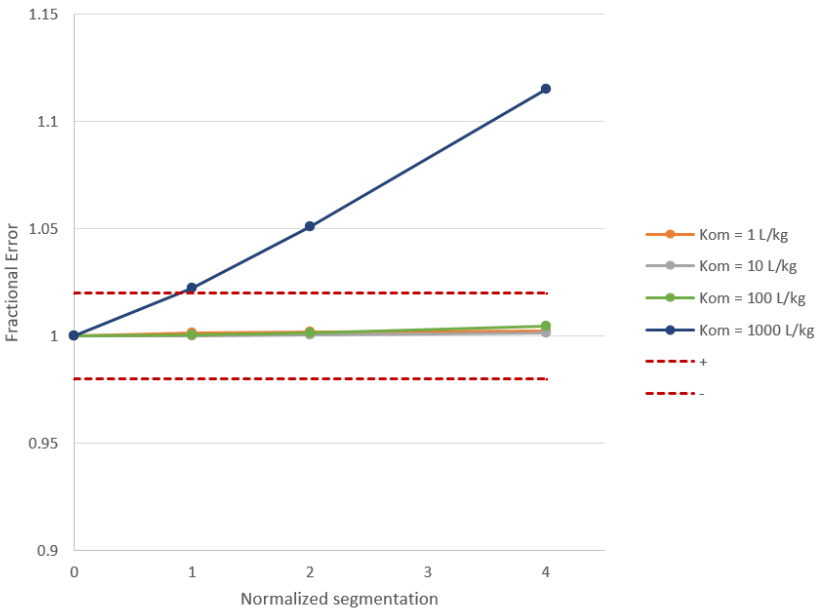

Figure A3b *PEC calculated for the different segmentations divided by continuum value for PEC as function of normalized segmentation for different values of Kom for standard segmentation.*

A3.6 Finer segments thicknesses for K_{om} > 100 000 L/kg

For K_{om} 1 000 000 L/kg, the applied segmentation G_1* did not give accurate results. An additional simulation can be run with a smaller segmentation ($G_{0.5}$*) to explore if more acceptable results would be obtained. This was done earlier for a slightly different scenario, the sediment properties (bulk density, organic matter content, porosity and tortuosity) differed (unpublished work). When running the simulation with the $G_{0.5}$* segmentation lower continuum values were obtained; the continuum value $f_{h=0}$* was lower than the continuum value calculated with f_1*, f_2*, f_3*. Hence, they differed but were consistent. Also the order of convergence decreased (which is positive), and the error, *e* and the error band, CGI. The fractional error for this segmentation, $A_{0.5}$* was still too high, which indicated that the $G_{0.5}$* segmentation was still not sufficiently fine to calculate PEC values for K_{om} 1 000 000 L/kg within 2% of a continuum value. For such substances, a finer segmentation is needed. The results obtained with a larger segmentation remain conservative.

A3.7 Continuum value accuracy and advised segmentation

The accuracy of the continuum values was evaluated by considering the *CGI* (≈bandwidth). The acceptable difference was again assumed to be 2%.

CGI and the considered acceptable bandwidth of 2% are provided in Table A7, for a fine segmentation and the standard segmentation. For both the fine- and the standard spacing for increasing K_{om} the CGI moves from lower than 2% to larger than 2 percent. The PEC calculated by GEM is for smaller Kom within the range of the $f_{h=0}$, but for larger K_{om} it becomes much higher for the standard segmentation, for the fine segmentation it stays within the indicated range of 2%.

For K_{om} 1000 L/kg, the continuum value calculated for the fine segmentation is higher than the continuum value calculated for the standard segmentation. This means that using coarser segmentation (even the most refined of those segmentations, G1) is not conservative (Figure A4). On the basis of this result it is advised to use the fine segmentation for calculations with K_{om} 1000 L/kg.

Table A6 *Continuum value for PEC (fh=0) with and error band (≈ grid convergence index, CGIfine) and acceptable error of 2% derived from PEC from the greenhouse soilless scenario with segmentation as given in Table 1 (fine) and 2 (standard) and for a range of Kom values of the substance in sediment. Values for which CGI bandwidth > 2% bandwidth are marked in yellow. (F = failed run, N = not considered further in the analysis).*

K_{om} (L/kg)	Fine		standard	
	$f_{h=0}$* ± CGI (µg/L)	$f_{h=0}$* ± 2% (µg/L)	$f_{h=0}$ ± CGI (µg/L)	$f_{h=0}$ ± 2% (µg/L)
1	F	F	697.5 ± 1.1	697.5 ± 14
10	F	F	689.9 ± 0.1	689.9 ± 13.8
100	F	F	649.5 ± 0.3	649.5 ± 13
1 000	536.2 ± 1	536.2 ± 10.7	527.9 ± 14.5	527.9 ± 10.6
10 000	372.1 ± 1.9	372.1 ± 7.4	N	N
100 000	176.9 ± 31.7	176.9 ± 3.5	N	N
1 000 000	43 ± 33.7	43 ± 0.9	N	N

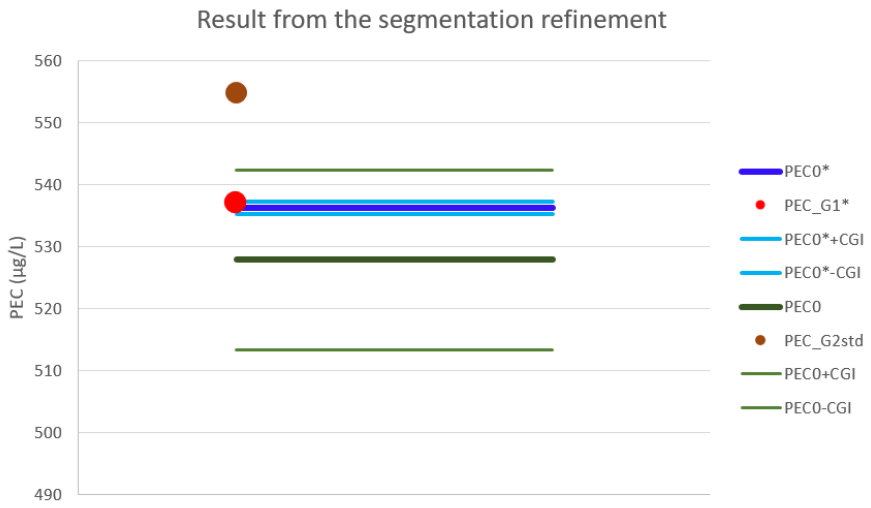

Figure A4 *PEC-f*h=0 (thick blue line), PEC-fh=0 (thick dark green line), PEC-f*h=0 ± CGI (thin blue lines), PEC-fh=0 ± CGI (thin green lines), PEC-f1* (red circle) and PEC-f2 (brown circle) for Kom 1000 L/kg.*

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