User's manual TOXSWA 1.2

Simulation of pesticide fate in small surface waters

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ABSTRACT

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TOXSWA is a computer model that simulates pesticide concentrations in the water and sediment layers of a water body. The theoretical concepts are briefly discussed. A sample simulation is presented to guide the user in running TOXSWA 1.2. The input and output files are described. The use of a graphical user interface for writing the input, running the program and creating the graphical output are discussed. Guidelines are given for estimating the input parameters.

Keywords: computer model, environmental protection, pesticide, surface water

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Contents

Preface

Agricultural use of pesticides may harm aquatic ecosystems. To predict negative effects a methodology is needed to estimate exposure concentrations for aquatic organisms. The Directorate of Science and Transfer of Knowledge of the Dutch Ministry of Agriculture, Nature Management and Fisheries asked the DLO Winand Staring Centre (SC-DLO) to develop such a methodology. By the end of 1991, the project 'Modelling transport routes and fate of pesticides in soil and field ditches' started at SC-DLO.

From the end of 1991 up to the middle of 1995 the project work took place within the framework of project 7242 of the DLO programme 147 'Ecotoxicological Risks of Pesticides in Aquatic and Terrestrial Ecosystems', financed by the Dutch Ministry of Agriculture, Nature Management and Fisheries. From the middle of 1995 onwards, the project has been financed both by the SC-DLO (SEO-project 597) and by the Ministry mentioned above (project 592 of DLO programme 276 'Emissions and Ecotoxicological Hazards of Pesticides').

The general administrative order on Environmental Admission Requirements for Pesticides (Ministry of Housing, Spatial Planning and Environment, 1995) mentions that the TOXSWA model is to be included in the risk assessment procedure in the Netherlands.

TOXSWA 1.0 was released with a user's manual (Beltman et al., 1996). This user's manual issued in 1999 accompanies TOXSWA 1.2. Version 1.2 has been used in the Dutch registration procedure since 1 June 1999. This manual has been written according to the guidelines developed by the Software Engineering Research Centre (SERC) in the framework of the software quality project at SC-DLO. The graphical user interface of TOXSWA 1.0 was developed in two steps by Mark van Elswijk of SERC and it was updated for TOXSWA 1.2 by Gerben van Laar of the Group Software Enginering of SC-DLO. A new feature of the Graphical User Interface (GUI) is the comparison of simulation results with experimental data.

In 1999 TOXSWA has been implemented in the Dutch registration procedure. Standard scenarios have been developed to be able to use the TOXSWA model in the authorization procedure of pesticides (Beltman and Adriaanse, 1999). The TOXSWA software can be obtained via the internet webpage of SC-DLO (http://www.sc.dlo.nl). The software includes the input files of the standard scenarios, and the Graphical User Interface (TOXSWA-GUI).

TOXSWA 2.0 is being developed to simulate the surface water scenarios of the EU FOCUS Workgroup, that are intended to be used in the harmonised pesticide registration procedure at EU level. TOXSWA is extended with the options of pesticide entries via drainage and runoff by coupling TOXSWA to other field scale models simulating drainage and runoff. Version 2.0 is to be released by the end of 1999.

Summary

This manual explains how to use the TOXSWA 1.2 simulation model on a PC. TOXSWA (TOXic substances in Surface WAters) is a computer model that simulates the concentrations of pesticides in the water and sediment layers of water bodies at the edge-of-field scale. Concentrations are calculated as a function of the geometry of the water body, the flow conditions, pesticide properties and types loading.

Version 1.2 of TOXSWA is confined to simulate a constant flow velocity and a constant water depth in the water body. Pesticide loadings may occur once or repeatedly by pulse inputs or distributed inputs into the water layer. An upward seepage of pesticides through the water body sediment may occur; this intends to simulate a drainage ditch.

Some brief background information on TOXSWA is provided. The entry routes of the pesticide, the processes modelled and a schematisation of the water body are presented.

An example of a TOXSWA run is provided that gives the user a first impression of how TOXSWA should be handled. Next, the input files for the water layer, the sediment, the hydrology and the pesticide are discussed. Then the output files are described that include concentrations, mass balances and the distribution of the pesticide between the compartments. This is followed by an introduction to the TOXSWA Graphical User Interface.

Information is provided on how to estimate input parameters for TOXSWA if no information is available or if the available information is incomplete.

Finally, the installation of TOXSWA is discussed.

1 Introduction

1.1 Scope of user's manual

The TOXSWA model (TOXic substances in Surface WAters) is a computer model that simulates concentrations of pesticides in the water and sediment layers of water bodies. Concentrations are calculated as a function of the geometry of the water body, the flow conditions, pesticide properties and types loading. Estimates of exposure concentrations are needed in the risk assessment procedure for aquatic ecosystems.

Version 1.2 of TOXSWA is confined to simulate a constant flow velocity and a constant water depth in the water body. Pesticide loadings may occur once or repeatedly by pulse inputs or distributed inputs into the water layer. An upward seepage of pesticides through the water body sediment may occur; this intends to simulate a drainage ditch.

This manual describes the TOXSWA software, version 1.2 for PC. It provides guidelines for preparing the input files, running the program and preparing graphical output with the aid of Graphical User Interface. A simulation with the Dutch standard scenario for spring is given as an example.

The theoretical concepts on which the model is based have only been briefly described. Adriaanse (1996) reported on the conceptual model, the numerical model and the model verification.

In comparison to TOXSWA 1.0, the main advances of TOXSWA 1.2 are:
- the implementation of temperature effects on transformation and volatilization (described in Section 2.5), and
- the possibility to simulate repeated applications instead of a single application at the start of the simulation.

Note that a difference between TOXSWA 1.0 and TOXSWA 1.2 is that in TOXSWA 1.0 nodes, indicating the middle of segments, were defined in the water layer (x axis) and sediment (z axis), while in TOXSWA 1.2 the user has to specify segments. The TOXSWA program still solves the mass conservation equations in the nodes, but the input has become easier to understand for the user.

In the user's manual of TOXSWA 1.0 (Beltman et al., 1996) we used the term *ditch*, the water body that TOXSWA has been developed for originally. In this manual we use the more general term *water body,* anticipating on the next version of TOXSWA (2.0) that will be able to simulate streams and ponds as well.

In this manual, TOXSWA is treated as a 'black box'. A future programmer's manual will discuss the structure of the program and present the vocabulary used.

1.2 Conditions of use and distribution

The DLO Winand Staring Centre supplies TOXSWA. It can be downloaded from the SC-DLO website (see Chapter 9). It is permitted to install and use TOXSWA on any of your computers at any time for the purpose of conducting scientific research. You may copy TOXSWA for your own use, but you may not:

- use, copy, decompile, reverse engineer, disassemble,
- modify or adapt TOXSWA, in whole or in part;
- create derivative works based upon TOXSWA in whole or part;
- remove any proprietary notices, labels or marks on TOXSWA;
- rent, lease, loan, sublicense, distribute or otherwise transfer TOXSWA in any form to any third party.

When publishing research results that have been accomplished through the use of TOXSWA, you shall explicitly acknowledge the use of TOXSWA in your publication.

Although any liability for damages resulting from errors is declined, you are kindly asked to report any errors or deficiencies. Other information or comments on TOXSWA 1.2 are welcomed as well.

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1.3 Structure of user's manual

This manual consists of nine chapters:
Chapter 1 provides a general introduction and some information on this user's manual.
Chapter 2 briefly describes the underlying concepts of TOXSWA, the limitations of TOXSWA and the TOXSWA program.
Chapter 3 helps you to make a first run with the model, for the example input that is automatically downloaded with TOXSWA 1.2.
Chapter 4 describes the input files for TOXSWA.
Chapter 5 describes the output files generated by TOXSWA.
Chapter 6 explains you how to handle TOXSWA-GUI.
Chapter 7 explains you how to do TOXSWA simulations.
Chapter 8 helps you to estimate the input parameters.
Chapter 9 provides information on the hardware and software requirements, and on the installation of the TOXSWA software.

Lines in the text printed in `courier` type represent what can be seen on the screen.

2 General description of TOXSWA

2.1 Introduction

Application of pesticides to agricultural fields may result in their entry into surface waters. In pesticide registration procedures the hazards of pesticides to aquatic organisms are commonly assessed by comparing estimated exposure concentrations in the field with laboratory toxicity data of some standard test organisms (algae, *Daphnia*, fish). TOXSWA (TOXic substances in Surface WAters) is developed to estimate acute and chronic exposure in water bodies. The model is to be used in the Dutch registration procedure (Ministry of Housing, Spatial Planning and Environment, 1995) and has been implemented in this procedure since 1 June 1999.

2.2 What is simulated by TOXSWA?

TOXSWA describes the fate of pesticides entering water bodies (i) by drift or atmospheric deposition, (ii) by surface runoff, or (iii) by drainage or leaching through the soil (see Fig. 1). Entries into the simulated system can be instantaneous or distributed over a certain period. The entries can emanate from a point or they can be distributed over a certain length of the water body.

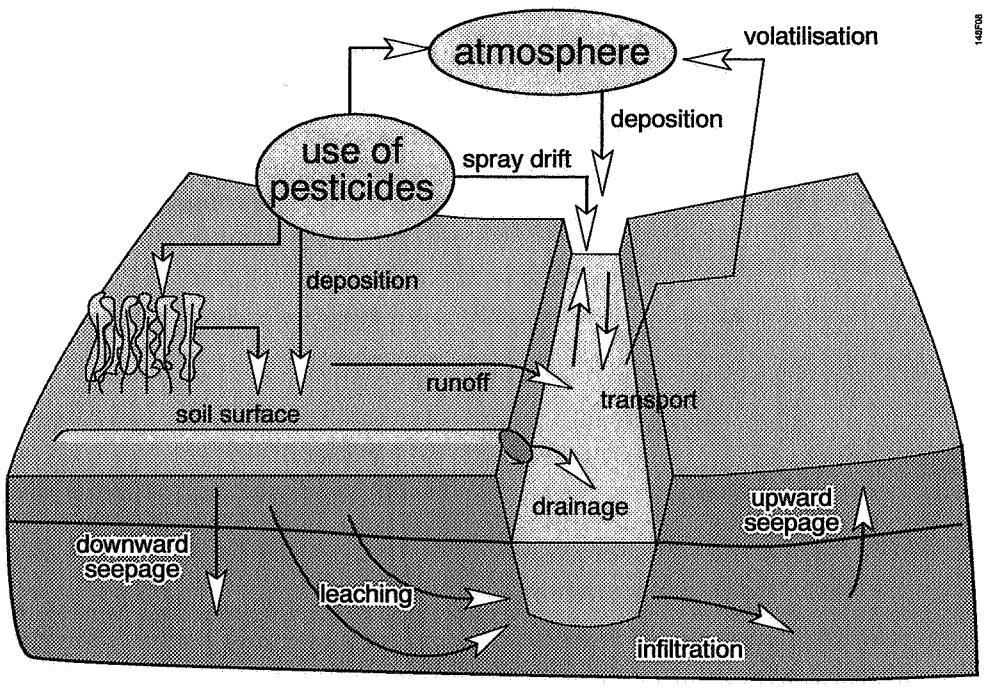

Fig. 1 Possible entry routes of pesticides into field ditches

The simulated water body system is two-dimensional and consists of two subsystems: a water layer containing suspended solids and macrophytes and a sediment layer whose properties (porosity, organic matter content and bulk density) vary with depth. The vertical cross section of the water subsystem has a trapezoidal shape (see Fig. 2). In the water layer subsystem, the pesticide concentration is assumed to be constant in the wetted cross section, so it is only a function of the horizontal direction. In the sediment subsystem, the pesticide concentration is a function of both the horizontal and vertical directions. Water and sediment exchange pesticide mass through the wetted perimeter of the water body.

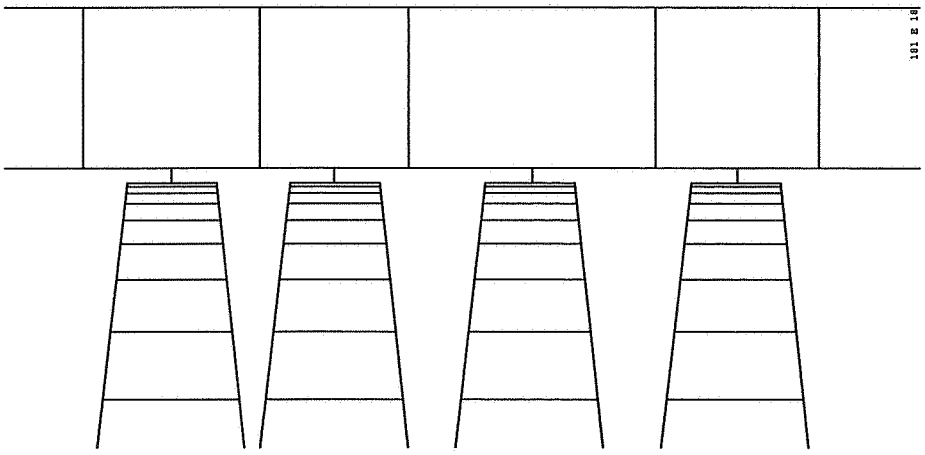

Fig. 2 Structure of the TOXSWA water body system: one water layer subsystem and many sediment subsystems

TOXSWA considers four processes: (i) transport, (ii) transformation, (iii) sorption and (iv) volatilization. In the water layer, pesticides are transported by advection and dispersion, whereas in the sediment, diffusion is included as well. The transformation rate covers the combined effects of hydrolysis, photolysis and biodegradation; metabolites are not considered. Sorption to suspended solids and to sediment is described using the non-linear Freundlich equation. Sorption to macrophytes is described using a linear isotherm. Pesticides are transported across the water-sediment interface by advection (upward or downward seepage) and by diffusion.

Mass balances for an elemental volume in the water layer and in the sediment link all the processes together; the mass balances result in two mass conservation equations. These two differential equations are solved using a generalized finite-difference method. For the numerical solution, the water layer subsystem is divided into a number of segments in the horizontal direction. Below each segment, a number of segments are defined for the sediment subsystem. Segment lengths in the water and sediment subsystems are of the order of metres and millimetres, respectively.

2.3 Temperature in TOXSWA

2.3.1 Introduction

Transformation and volatilization are the most important processes in TOXSWA 1.0 (Westein et al., 1998). In TOXSWA 1.0 (Adriaanse, 1996; Adriaanse, 1997; Beltman et al., 1996) it is implicitly assumed that the temperature in the water body is 20 °C, because transformation and volatilization parameters have been determined at 20 °C. TOXSWA 1.2 has been extended to include the effect of temperature on transformation and volatilization.

Process descriptions for the dependency of transformation on temperature are given by Boesten (1986) and for the dependency of parameters determining volatilization by Van den Berg and Boesten (1998). Their equations were incorporated in TOXSWA 1.2 (Section 2.3.2). The temperature in TOXSWA is constant in time, so seasonal or daily variations are not (yet) simulated.

The standard scenarios developed for TOXSWA 1.0 (Beltman and Adriaanse, 1999) contained no temperatures. Therefore temperatures for the spring and autumn scenario are derived in Section 2.3.3. The consequences of implementing the temperature in TOXSWA for the exposure concentrations of the standard scenarios (including the standard graphs) are discussed in Section 2.3.4.

2.3.2 Transformation and volatilization

The rate coefficient for the transformation of the substance depends on the temperature. The Arrhenius equation was developed to describe the effect of temperature on the rate coefficient of a chemical reaction. Walker (1974) proposed to describe the temperature dependency of the transformation rate coefficient in soil with the Arrhenius equation. The equation is not necessarily applicable to the combination of chemical and microbial transformation processes. There is no theoretical base for using the equation for microbial transformation. Nevertheless, Boesten (1986) concluded from a literature compilation that the Arrhenius equation gave a good description of experimental data. With the aid of the Arrhenius equation the transformation rate coefficient at a temperature T can be derived from the transformation rate coefficient at a reference temperature T_{ref} with:

$$k(T) = k(T_{ref}) \exp\left[\frac{E}{R \cdot T_{ref} \cdot T}\left(T - T_{ref}\right)\right] \qquad (1)$$

where:

T	=	temperature (K)
T_{ref}	=	reference temperature (K)
k	=	transformation rate coefficient (d^{-1})
E	=	molar Arrhenius activation energy (J mol^{-1})
R	=	universal gas constant (≈ 8.3144 J mol^{-1} K^{-1})

The FOCUS Soil Modelling Workgroup (1997) found an average value of the molar Arrhenius activation energy of 55 kJ mol^{-1} (S.D. 15 kJ mol^{-1}) for about 50 experiments covering a range of pesticides and soils. The whole range covered 20 to 100 kJ mol^{-1}.

Note that all evidence for the applicability of Eq. (1) and all values for E were determined for soil. In surface waters additional processes as photolysis may occur, and in sediments anaerobic conditions may affect microbial transformation in an indirect way. Hence, further research should be done on the temperature dependency of transformation in water and sediment.

In TOXSWA volatilization is calculated using the Henry coefficient (Adriaanse, 1996). The temperature dependency of this coefficient can be calculated from the temperature dependency of the saturated vapour pressure and of the water solubility.

The dependency of the saturated vapour pressure on the temperature is derived from the Van 't Hoff equation via:

$$P(T) = P(T^{ref}) \exp\left[\frac{\Delta H_P}{R}\left(\frac{1}{T} - \frac{1}{T^{ref}}\right)\right] \qquad (2)$$

(Van den Berg and Boesten, 1998), with:

P = saturated vapour pressure of substance (Pa)

ΔH_P = enthalpy of vaporization (J mol^{-1})

The enthalpy of vaporization depends on the substance. Smit et al. (1997) estimated an average enthalpy of vaporization of 95 kJ mol^{-1} from literature data on 16 pesticides (range: 58 to 146 kJ mol^{-1}). The saturated vapour pressure is a basic physical property of the substance; hence the average estimated by Smit et al. (1997) is valid for surface water as well. We suggest using 95 kJ mol^{-1} as the default value, when no value is available.

The effect of the temperature on the water solubility is derived from the Van 't Hoff equation via:

$$C_{sol}(T) = C_{sol}(T_{ref}) \exp\left[-\frac{\Delta H_{sol}}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right] \qquad (3)$$

(Van den Berg and Boesten, 1998), with:

c_{sol} = solubility of substance in water (g m^{-3})

ΔH_{sol} = enthalpy of dissolution (J mol^{-1})

The enthalpy of dissolution depends on the substance. For most pesticides an enthalpy of dissolution of 27 kJ mol^{-1} can be taken as default value. Bowman and Sans (1985) found a range of -17 to 156 kJ mol^{-1}.

Note that using the default values 95 and 27 kJ mol^{-1} implies that the Henry coefficient increases with temperature, corresponding to an activation energy of 68 kJ mol^{-1}.

2.3.3 Standard scenarios

The standard scenarios proposed in Beltman and Adriaanse (1999) for the Dutch registration procedure represent a spring/summer and an autumn situation. For both scenarios a temperature characterising the standard ditch has to be selected. For the spring/summer scenario a spring temperature will be used, being lower than that in summer, and therefore representing the 'worst case' situation.

The KNMI (1992) published average air temperatures in the Netherlands for spring and summer over the period 1961-1990. The average air temperature in spring at 1.5 m above the soil surface was 8.3 °C (range: 4.0 to 12.4 °C), and in autumn it was 10.3 °C (range: 6.7 to 13.8 °C).

At the SC-DLO experimental ditches the air temperature and water temperature (10 cm below the water surface) were measured. In 1989, the air and water temperatures were averaged over the whole spring period (March to May) and over the whole autumn period (September to November). For both seasons the average air temperature differed less than 1 °C from the average water temperature (Personal communication, J. Drent SC-DLO, 1999).

Therefore, we propose to characterise the water in the standard ditch by a temperature of 10 °C in the spring as well in the autumn scenario.

2.3.4 Consequences for calculation of exposure concentrations

Compared to TOXSWA 1.0, additional parameters for temperature, transformation and volatilization have to be entered. The main difference with simulations done by TOXSWA 1.0 is the longer half-life for transformation in the water layer at 10 °C in the standard ditch now, compared to 20 °C of TOXSWA 1.0. The concentrations in the water layer and in the sediment decrease slower. A decrease of 10 °C doubles the half-life (Mensink et al., 1995), and consequently also the exposure concentrations will be twice as high as those simulated by TOXSWA 1.0. The impact of the temperature on the volatilization is in the same order as its impact on transformation. An increase of the temperature with 10 °C increases in the Henry coefficient approximately by a factor 2.5, and so does the volatilization rate.

The standard graphs presented in Beltman and Adriaanse (1999) give the momentary concentration and the time weighed average exposure concentrations as a function of the overall dissipation half-life. By implementing the temperature in TOXSWA 1.2 and in the standard scenarios, the calculation of the overall dissipation half-life needs an additional step compared to the procedure given by

Beltman and Adriaanse (1999). In the additional step, the half-life for transformation in the water layer at the reference temperature of 20 °C is replaced by the half-life for transformation at the scenario temperature of 10 °C, using Eq. (1). The Henry coefficient needs to be calculated at 10 °C as well. Next, the transformation half-life at 10 °C and the Henry coefficient at 10 °C are used to calculate the overall dissipation half-life at 10 °C, which can be used to estimate the exposure concentrations from the standard graphs.

2.4 Limitations of TOXSWA

TOXSWA was developed to estimate exposure concentrations of aquatic organisms in ditches, implying that it was not meant to simulate large water bodies like lakes or rivers. Neither is TOXSWA designed for simulations on a regional scale.

In the current registration procedure, chronic exposure of organisms to pesticides is tested in laboratory tests executed for a maximum of 28 days. Originally, this was also the time period TOXSWA has been developed for. That is the reason we did not include formation of additional sediment by sedimentation of suspended solids. So, increases in sediment thickness and deposition of suspended solids on the bottom have not been incorporated in TOXSWA. Resuspension was not included as well. TOXSWA 1.2 may be applied for periods of up to 200 d. One should, however, be aware of the limitations of the suspended solids behaviour described above.

The sediment has been divided into subsystems in the direction of flow in the watercourse. These subsystems are composed of thin horizontal layers (segments), in which pesticide concentrations are calculated, determined by the pesticide concentrations in the overlying water layer. It has been assumed that lateral interaction between the sediment subsystems does not occur.

The sediment is vertically subdivided, but lateral interaction between the separate sediment subsystems is not modelled.

TOXSWA 1.0 does not include the possible variation of transformation rate in time caused by e.g. changes in acidity and intensity of light. In estimating the parameters for transformation, one should keep in mind for which period one wants to characterise to obtain a 24 h representative transformation rate. One may e.g., average the transformation parameters determined with and without light, weighing them for the duration of the day and night.

It should be stressed that TOXSWA is a model, hence a simplification of reality. One should therefore always be cautious when drawing conclusions from the simulation results. Keep in mind that the quality of the model results is limited by the quality of the input data. Therefore, careful selection of the input data is of utmost importance. As a general rule, one should not simulate the fate of pesticides in ditches with the aim of obtaining realistic concentrations without

accompanying experiments in the laboratory and or field. Experiments are needed to obtain site-specific parameters and to calibrate and verify the results of model simulations.

New in TOXSWA 1.2 is that repeated applications can be simulated.

2.5 Program evaluation

A limited verification of the program has been done by comparing results of TOXSWA simulations with analytical solutions (Adriaanse, 1996). Concentrations in the water layer calculated by TOXSWA agreed perfectly with the concentrations calculated with an analytical solution for the water layer after a pulse input. A pulse input in the sediment resulted also in a perfect agreement between concentrations calculated by TOXSWA and concentrations calculated by the analytical equation.

The sensitivity analysis of TOXSWA 1.0 of Westein et al. (1998) demonstrated that three system parameters determine almost completely the exposure concentration of a specified pesticide. The parameters are water depth, flow velocity and macrophyte mass. They also demonstrated that the rate coefficient for transformation in the water layer and the Henry coefficient (indicating volatilization) are the pesticide properties that determine mainly the exposure concentrations.

TOXSWA 1.2 will be tested using three data sets of experiments with chlorpyrifos, carbendazim and linuron respectively, carried out in microcosms (1 m^3) (Westein et al., in preparation). Two experiments in the outdoors experimental ditches of SC-DLO resulted in two other data sets that are planned to be used for validation purposes. One data set concerns the fate of the insecticide chlorpyrifos in the ditch with no flow through. The second data set is on the fate of linuron, sprayed three times at monthly intervals, for a water flow of about 5 m d^{-1}.

3 Getting started

This chapter explains how to make a simulation run with the TOXSWA program using the TOXSWA-GUI and how to obtain the graphs presenting the simulation results. Before you start, make sure the software has been properly installed on your computer (see Chapter 9).

The example input concerns spray drift deposition of the pesticide chlorpyrifos onto the water surface, for the Dutch standard scenario for spring. Chlorpyrifos sorbs strongly to suspended solids and the sediment ($K_{om,ss}$ = $K_{om,wb}$ = 16 400 L kg^{-1}). The values of all parameters can be found in the eleven input files of this example shown in Figures 3-13. In Chapter 4 these input files are discussed into more detail.

Start the TOXSWA-GUI (Graphical User Interface of TOXSWA) by clicking the TOXSWA icon. When you did not make a shortcut to your computer desktop; click ToxswaGUI.EXE in `c:\toxswa\gui` to start the GUI. Now, you are on the main page (or TOXSWA page) of the GUI.

The white boxes within the "Run" section show you which scenario and which pesticide is considered by the GUI. By default, the Dutch standard scenario for spring (`NLstandard_SP`) and the example pesticide chlorpyrifos (`Cpf`) are shown. By using the Windows Explorer, the input files defining the scenario can be found in directory `c:\toxswa\scenarios\NLspring_SP`, and the input file defines the pesticide in directory `c:\toxswa\pesticides\Cpf`.

To run the example, click the "Run TOXSWA" button. The simulation may take a some time (see Chapter 9). Thirty days are simulated. The progress of the simulation is shown in the DOS-box that is present at your screen during the simulation. After the simulation is finished the DOS-box echoes:

```
    end of simulation
Stop - Program terminated
```

In the directory `c:\toxswa\runs\NLstandard_SP+Cpf` 21 output files have been created. Examples of these output files are shown in Figures 14-26 in Chapter 5, where the contents of the output files are discussed.

To view the graphs that the GUI generates from the data in the output files, click the "View output" button. Five graphs can be shown by the GUI. Select one of them by marking the corresponding radio button. Clicking "View" then gives the selected graph. Use the close button on the right at the bottom of the page (open door with red triangle) to go back to the previous screen. The "Concentration of pesticide in time" graph also contains a table presenting the exposure concentrations.

4 Description of input files

4.1 Introduction

The input of the program is organized in eleven input files. The files are :

WLNU.INP	water layer; numerical, spatial and temporal discretisation
WLPA.INP	water layer; time-independent parameters
WLST.INP	water layer; initial concentrations per segment
WBNU.INP	sediment; numerical, spatial and temporal discretisation
WBPA.INP	sediment; time-independent parameters
WBST.INP	sediment; initial concentrations per segment
HY.INP	hydrology; flow in water body, seepage/infiltration through sediment
SL.INP	substance loadings, time, mass, entry length
SU.INP	substance properties; sorption, transformation, volatilization
FILES.INP	names and paths of the input files
OPOUT.INP	output options; which files, times and sediment subsystems

Note that the names of files concerning the water layer start with the letters WL, and the names of the files concerning the sediment with the letters WB. These acronyms are based on the Dutch names for the water layer and the sediment.

Annex 1 presents a table describing each parameter in the input files, including names, units and data type in the program.

The input files are discussed in the sections below. The examples of the input files described concern the example presented in Chapter 3. In the input files the units and the permitted range are shown for each parameter value.

The parameters of the conceptual model described by Adriaanse (1996), have been indicated in *italics* between brackets where relevant.

4.2 Water layer

4.2.1 WLNU.INP

This file contains data for the numerical solution including the discretisation of the water layer, and the time parameters. The number of lines depends on the number of segments defined in the file. Figure 3 shows an example of WLNU.INP.

Section 1
The numerical weight factors for space (β) and time (θ) respectively, indicate how the mass conservation equations will be solved. The finite difference method is applied in fully forward form if the value of the weight factor for space is 0. For the maximum value of 1, the solution method is fully backwards. The weight factor for

time ranges from 0, defining a fully implicit difference scheme, to 1 defining a fully explicit scheme. The solution method is intermediate to these two extremes for weight factors between 0 and 1. In version 1.2 of TOXSWA the values of β and θ are fixed on 0.5 and 1.0, respectively, for both the water layer and the sediment, resulting in an explicit central difference calculation scheme.

Section 2
The selected time step for the water layer should be equal to that of the sediment. The total simulation time (in days) applies to the sediment as well.

Sections 3, 4 and 5
The lengths of the water body and its front and end buffers have to be entered as well as the corresponding number of segments per unit of length (water body: *nxsexdit* segments; front buffer: *nxsefb* segments; end buffer: *nxseeb* segments). The maximum total number of segments (*nxsexdit+nxsefb+nxseeb*) that the program can handle is 25+500+25. In version 1.2 of TOXSWA, the length of the buffers has been fixed at zero, because the constant water flow in the water body makes the buffers superfluous (the buffers prevent numerical problems when the direction of the water flow may become reversed during the simulation).The cumulative lengths of the segments have to equal the total length of the water body. The number of lines used to describe the segment lengths depends on the number of segments in the water body.

```
*
*   TOXSWA input file
*   GUI version: 1.0
*
*   Filename: C:\TOXSWA\SCENARIOS\NLStandard sp\WLNU.INP
*   Contents: Input data for TOXSWA concerning numerical solution and
*             time and length of water body considered
*   Date    : 2/10/99
*
*-------------------------------------------------------------------------------
*
*   Section 1: Numerical weight factors
*-------------------------------------------------------------------------------
*
*   numerical weight factor for space
  betawl = 0.5                    ! unit: -          range: 0. .... 1.
*   numerical weight factor for time
  thetawl = 1.                    ! unit: -          range: 0. .... 1.
*
*-------------------------------------------------------------------------------
*
*   Section 2: Time parameters
*-------------------------------------------------------------------------------
*
*   selected time step for water layer (multiple should equal one day)
  deltwl = 600.                   ! unit: s          range: 1. .... 86400.
*   total time considered (holds also for sediment)
  ttot = 30.                      ! unit: d          range: 0.1 .... 500.
*
```

Fig. 3 Example of a WLNU.INP file

```
*-------------------------------------------------------------------------------
*
*   Section 3: Space parameters
*-------------------------------------------------------------------------------
*
*   total length of water body considered
  xdit = 320.                    ! unit: m          range: 0.05 .... 10000.
*   length of front buffer (0. if none)
  xfb = 0.                       ! unit: m          range: 0. .... 1000.
*   length of end buffer (0. if none)
  xeb = 0.                       ! unit: m          range: 0. .... 1000.
*-------------------------------------------------------------------------------
*
*   Section 4: Number of segments
*-------------------------------------------------------------------------------
*
*   number segments in water body
  nxsedit = 80                   ! unit: -          range: 1 .... 500
*   number segments in front buffer (0 if none)
  nxsefb = 0                     ! unit: -          range: 0 .... 25
*   number segments in end buffer (0 if none)
  nxseeb = 0                     ! unit: -          range: 0 .... 25
*-------------------------------------------------------------------------------
*
*
*-------------------------------------------------------------------------------
*
*   Section 5: Lengths of segments
*-------------------------------------------------------------------------------
*
*   lengths of segments in front buffer (0. if none)
  lesefb = 0.                    ! unit: m        range: 0. .... 1000.
*   lengths of segments in water body
 lesedit =    4.    4.    4.    4.    ! unit: m   range 0.05 .... 1000.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
              4.    4.    4.    4.
*   lengths of segments in end buffer (0. if none)
  leseeb = 0.                    ! unit: m          range: 0. .... 1000.
*
*----END OF FILE--------------------------------------------------------------
```

(continuation of Fig 3)

4.2.2 WLPA.INP

This file contains time-independent data for the water layer such as the geometry of the water body, amount of suspended solids and macrophytes. See Figure 4 for an example of WLPA.INP.

```
*
*   TOXSWA input file
*   GUI version: 1.0
*   TOXSWA version: 1.2
*
*   Filename: C:\TOXSWA\SCENARIOS\NLStandard_sp\WLPA.INP
*   Contents: Input data for TOXSWA concerning geometry and other
*             characteristics of the waterbody
*   Date    : 4/21/99
*
*-------------------------------------------------------------------------------
*
*   Section 1: Geometry of the waterbody
*-------------------------------------------------------------------------------
*
*   bottom width of waterbody
  wibot = 0.4                    ! unit: m          range: 0.05 .... 100.
*   side slope, horizontal/vertical
  sisl = 1.                      ! unit: m          range: 1.E-5 .... 10.
*   water depth defining perimeter for exchange water layer - sediment,
*   h_w
  wdhfl = 0.1                    ! unit: m          range: 0. .... 2.
*
*-------------------------------------------------------------------------------
*
*   Section 2: Geometry of the neighbouring plot of land
*-------------------------------------------------------------------------------
*
*   length of draining plot perpendicular to waterbody and located
*   at one or both sides
  leplot = 999.                  ! unit: m^2/d      range: 10. .... 100000.
*
*-------------------------------------------------------------------------------
*
*   Section 3: Concentration and organic matter in suspended solids
*-------------------------------------------------------------------------------
*
*   concentration of suspended solids, ss
  coss = 15.                     ! unit: g/m3       range: 1. .... 100000.
*   mass ratio of organic matter, m_om, ss
  raomss = 0.5                   ! unit: -          range: 0. .... 1.
*
*-------------------------------------------------------------------------------
*
*   Section 4: Amount of macrophytes
*-------------------------------------------------------------------------------
*
*   dry weight of macrophyte biomass per m^2 bottom, DW
  dwmp = 0.                      ! unit: g/m^2      range: 0. .... 1000.
*
*----END OF FILE--------------------------------------------------------------
```

Fig 4 Example of a WLPA.INP file

Section 1
The side slope (s_1) defines the slope of the walls of the watercourse as the watercourse is the tangent, the horizontal distance divided by the vertical distance (Fig. 6 in Adriaanse,1996). The water depth-defining perimeter (h_w) defines which parts of the walls of the water body have to be taken into account for exchange between water layer and sediment. It should be larger than 0 and smaller than the water depth in the water body. The water depth in the water body (h) has to be entered in HY.INP.

Section 2
The length of the draining plot perpendicular to the water body (l) is of importance if seepage through the sediment occurs. The location of the plot, on one or on both sides of the watercourse, does not matter, as long as the length of the plot contributing to the seepage flow, is correct.

Sections 3 and 4
The concentration of the suspended solids (*ss*), its organic matter content ($m_{om,ss}$), and the dry weight of the macrophyte biomass per m^2 at the water body bottom (*DW*) have to be entered.

4.2.3 WLST.INP

This file contains the initial concentration (c) in every segment of the water layer, and the concentration pesticide in the air. Figure 5 shows an example of WLST.INP.

Section 1
The number of lines for the initial concentration in the water layer (c^*) depends on the number of segments (*nxsexdit+nxsefb+nxseeb*) defined. For a point-type contamination, all initial concentrations should be made zero, except for the one contaminated segment. For a distributed contamination (e.g. from spray drift) a row of segments in the water layer should receive an initial concentration, to be calculated from the loading at the water surface. Section 8.3 presents a method to calculate concentrations from the mass deposited on the water surface.

Section 2
The concentration in the air (c_a) is used to determine the concentration gradient between the water phase and the atmosphere in order to calculate the volatilisation through the water surface. In the absence of data, we generally select c_a to be zero.

```
*
*   TOXSWA input file
*   GUI version: 1.0
*
*   Filename: C:\TOXSWA\SCENARIOS\NLStandard_sp\WLST.INP
*   Contents: Input data for TOXSWA concerning initial concentrations
*             in the water layer
*   Date    : 2/10/99
*
*-------------------------------------------------------------------------------
*
*   Section 1: Initial concentrations
*-------------------------------------------------------------------------------
*
*   initial (start) mass concentration of pesticide in water layer, c**,
*   for segments in x-direction (nxsetot, so buffers included)
  castwl =    0.    0.    0.    0.    ! unit: g/m^3      range 0. .... 100.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
              0.    0.    0.    0.
*
*-------------------------------------------------------------------------------
*
*   Section 2: Constant background concentration in air
*-------------------------------------------------------------------------------
*
*   constant background concentration of pesticide in air
  coair = 0.                    ! unit: g/m^3      range: 0. .... 0.
*
*----END OF FILE--------------------------------------------------------------
```

Fig. 5 Example of a WLST.INP file

4.3 Sediment

4.3.1 WBNU.INP

This file contains data concerning the numerical solution including the discretisation of the sediment and the time parameters. The number of lines in this file depends on the number of segments that is defined in the sediment. Figure 6 shows an example of WBNU.INP.

Section 1

The numerical weight factors for the sediment, β for space and θ for time respectively, indicate how the mass conservation equation for the sediment will be solved. See the description of WLNU.INP for a discussion of the values of the parameters. In version 1.0 to version 1.2 of TOXSWA the values of β and θ are

fixed on 0.5 and 1.2, respectively, for both the water layer and the sediment, resulting in an explicit central difference calculation scheme.

```
*
*   TOXSWA input file
*   GUI version: 1.0
*
*   Filename: C:\TOXSWA\SCENARIOS\NLStandard sp\WBNU.INP
*   Contents: Input data for TOXSWA concerning numerical solution and
*             considered thickness sediment
*   Date    : 2/10/99
*
*-------------------------------------------------------------------------------
*
*   Section 1: Numerical weight factors
*-------------------------------------------------------------------------------
*
*   numerical weight factor for space
  betawb = 0.5                    ! unit: -          range: 0. .... 1.
*   numerical weight factor for time
  thetawb = 1.                    ! unit: -          range: 0. .... 1.
*
*-------------------------------------------------------------------------------
*
*   Section 2: Time parameters
*-------------------------------------------------------------------------------
*
*   selected time step sediment
  deltwb = 3600.                  ! unit: s          range: 1. .... 86400.
*
*-------------------------------------------------------------------------------
*
*   Section 3: Space parameters
*-------------------------------------------------------------------------------
*
*   length sediment considered (end buffer excluded)
  zwb = 0.1                       ! unit: m          range: 0.001 .... 0.5
*   length end buffer sediment (0. if none)
  zebb = 0.                       ! unit: m          range: 0. .... 0.1
*
*-------------------------------------------------------------------------------
*
*   Section 4: Number segments
*-------------------------------------------------------------------------------
*   number segments in sediment (end buffer excluded)
  nzsewb = 14                     ! unit: -          range: 1 .... 50
*   number segments in end buffer (0 if none)
  nzseebb = 0                     ! unit: -          range: 0 .... 10
*-------------------------------------------------------------------------------
--
*
*   Section 5: Thickness segments
*-------------------------------------------------------------------------------
*
*   thickness of segments in sediment
 lesewb =  0.001 0.001 0.001   ! unit: m          range 0.0001 .... 0.6
           0.001 0.002 0.002
           0.002 0.005 0.005
            0.01  0.01  0.02
            0.02  0.02
*
*   thickness of segments in end buffer (0. if none)
  leseebb = 0.                    ! unit: m          range: 0. .... 0.6
*
*----END OF FILE--------------------------------------------------------------
```

Fig. 6 Example of a WBNU.INP file

Section 2
In version 1.2 of TOXSWA the size of the time step (in s) for the sediment should be equal to the size of the time step in the water layer.

Section 3, 4 and 5
The thickness of the sediment layer and of the end buffer as well as the corresponding number of segments for the sediment and its end buffer (sediment: *nzsewb* segments; end buffer: *nzsebb* segments) have to be entered. The maximum number of segments (*nzsewb+nzsebb*) that the program can handle is 50+10. At the boundary between the water layer and the sediment $z = 0$; from there, the z co-ordinate increases with depth. The sum of the segment thicknesses must be equal to the total thickness of the sediment plus the end buffer. The number of lines required to describe the segments depends on the number of segments defined.

4.3.2 WBPA.INP

This file contains time-independent data for the sediment (see Fig. 7).

Sections 1 and 2
The bulk density of dry sediment material (ρ_b) is given for nzsewb segments, followed by the porosity (ε) and the tortuosity (λ), starting with the top segment. Section 2 contains the mass ratio of organic matter to dry sediment material ($m_{om,wb}$); the maximum value is 1. These parameters need not to be entered for the end buffer.

Section 3
Finally, the dispersion length for the sediment (E_{lb}) should be entered.

```
*
*   TOXSWA input file
*   GUI version: 1.0
*
*   Filename: C:\TOXSWA\SCENARIOS\NLStandard_sp\WBPA.INP
*   Contents: Input data for TOXSWA concerning sediment
*             characteristics
*   Date    : 2/10/99
*
*-------------------------------------------------------------------------------
*
*   Section 1: Physical properties sediment
*-------------------------------------------------------------------------------
*
*   bdwb(1-nzsewb), bulk density dry sediment material, rho_b (as a
*   function of depth, end buffer excluded)
*
*   por(1-nzsewb), porosity (volume fraction void water), epsilon (as
*   a function of depth, end buffer excluded)
*
*   tor(1-nzsewb), tortuosity, lamba (as a function of depth, end buffer
*   excluded)
*
  bdwb                por                 tor
    80.               0.82                0.82
    80.               0.82                0.82
    80.               0.82                0.82
    80.               0.82                0.82
    80.               0.82                0.82
    80.               0.82                0.82
    80.               0.82                0.82
   220.               0.77                0.77
   220.               0.77                0.77
   670.               0.62                0.62
   670.               0.62                0.62
  1500.               0.36                0.28
  1500.               0.36                0.28
  1500.               0.36                0.28
! kg/m^3              -                   -          unit
! 10. .... 3000.     0. .... 1.          0. .... 1.   range
*
*-------------------------------------------------------------------------------
*
*   Section 2: Organic matter sediment
*-------------------------------------------------------------------------------
*
*   mass ratio organic matter of dry sediment material, m_om,wb (as a
*   function of depth, end buffer excluded)
  racomwb = 0.25                ! unit: -         range: 0. .... 1.
            0.25
            0.25
            0.25
            0.25
            0.25
            0.25
            0.19
            0.19
            0.06
            0.06
            0.02
            0.02
            0.02
*
*-------------------------------------------------------------------------------
*
*   Section 3: Dispersion in sediment
*-------------------------------------------------------------------------------
*
*   dispersion length
  ldis = 0.015                  ! unit: m         range: 0. .... 1.
*
*-----END OF FILE--------------------------------------------------------------
```

Fig. 7 Example of a WBPA.INP file

4.3.3 WBST.INP

Section 1
This file contains the initial concentration (c_b*) for every segment in the sediment (see Fig. 8). The number of lines for the initial concentration in the sediment layer depends on the number of segments (*nznowbt+nznobb*) defined. Note that they are the total concentrations of pesticide, present at either the solid phase or in the liquid phase of the sediment.

```
*
*   TOXSWA input file
*   GUI version: 1.0
*
*   Filename: C:\TOXSWA\SCENARIOS\NLStandard_sp\WBST.INP
*   Contents: Input data for TOXSWA concerning initial concentrations
*             in sediment
*   Date    : 2/10/99
*
*-------------------------------------------------------------------------
*
*   Section 1: Initial concentrations
*-------------------------------------------------------------------------
*
*   Initial (start) mass concentration pesticide in sediment, c**,
*   for the total number of segments in z-direction (nzsetot, so end
*   buffer included
  castwb = 0.                    ! unit: g/m^3      range: 0. ..., 1000.
           0.
           0.
           0.
           0.
           0.
           0.
           0.
           0.
           0.
           0.
           0.
           0.
           0.
*
*----END OF FILE-------------------------------------------------------
```

Fig. 8 Example of a WBST.INP file

4.4 Hydrology: HY.INP

The HY.INP file contains data on the water flow in the water body and infiltration/seepage through the sediment (see Fig. 9).

Section 1
The constant water depth in the water body (h) is the thickness of the water layer. It should not be confused with the water depth defining perimeter (h_w) in WLPA.INP, which indicates which parts of the walls of the water body has to be taken into account for the exchange between water layer and sediment.

Section 2
The dispersion coefficient for the water layer (E_x) has to be entered.

Section 3
A constant seepage/infiltration flow from the neighbouring lot (q) into the water body (negative values) or out of the water body (positive values) has to be entered. The concentrations of the incoming water (c_{lot} entering the deepest sediment segment from below) should also be entered.

```
*
*   TOXSWA input file
*   GUI version: 1.0
*
*   Filename: C:\TOXSWA\SCENARIOS\NLStandard_sp\HY.INP
*   Contents: Input data for TOXSWA concerning hydrological
*             characteristics
*   Date    : 2/10/99
*
*-------------------------------------------------------------------------------
*
*   Section 1: Flow velocity and water depth of water layer
*-------------------------------------------------------------------------------
*
*   constant flow velocity in water body
  u = 10.                          ! unit: m/d        range: -100000. .... 
100000.
*   constant water depth in water body
  wdh = 0.3                        ! unit: m          range: 0.01 .... 2.
*
*-------------------------------------------------------------------------------
*
*   Section 2: Dispersion coefficient
*-------------------------------------------------------------------------------
*
*   dispersion coefficient of pesticide in water, E_x
  kds = 20.                        ! unit: m^2/d      range: 1. .... 100000000.
*
*-------------------------------------------------------------------------------
*
*   Section 3: Seepage with concentration
*-------------------------------------------------------------------------------
*
*   upward seepage through sediment into water body
  qseif = 0.                       ! unit: m^3/m^2.d  range: 0. .... 0.01
*
*   concentration of pesticide in incoming water
  colot = 0.                       ! unit: g/m^3      range: 0. .... 1.
*
*-------------------------------------------------------------------------------
*
*   Section 4: Temperature
*-------------------------------------------------------------------------------
*
*   temperature in water and sediment
  te = 283.                        ! unit: K          range: 273. .... 323.
*
*----END OF FILE--------------------------------------------------------------
```

Fig. 9 Example of a HY.INP file

4.5 Loadings: SL.INP

SL.INP contains data on substance loadings into the water layer (see Fig. 10).

Section 1
The entry route and source of data have to be selected.

```
*
*   TO*   TOXSWA input file
*   GUI version: 1.0
*
*   Filename: C:\TOXSWA\SCENARIOS\NLStandard_sp\SL.INP
*   Contents: Input data for TOXSWA concerning substance
*             loadings to the water layer via different entry routes
*   Date     : 2/10/99
*
*------------------------------------------------------------------------------
*
*   Section 1: Source of data and entry route
*------------------------------------------------------------------------------
*
*   switches for: user specified or model output, and type of entry route
*   (0 = no, 1 = yes), different sources of data and entry routes
*   can be combined
*
*   user specified, spray drift
  op_slus = 1                      ! unit: -           range: 0 .... 1
*   user specified, drainage
  op_slud = 0                      ! unit: -           range: 0 .... 1
*   user specified, runoff
  op_slur = 0                      ! unit: -           range: 0 .... 1
*   model output, drainage
  op_slmd = 0                      ! unit: -           range: 0 .... 1
*   model output, runoff
  op_slmr = 0                      ! unit: -           range: 0 .... 1
*
*------------------------------------------------------------------------------
*
*   Section 2: If op_slus = 1 (user specified, spray drift) specify:
*------------------------------------------------------------------------------
*
*   number of loadings  (max. of 500)
  ntslus = 1
*
*   tslus, time of loading (d)
*
*   mslus, mass per square metre (g/m^2) deposited onto the water surface
*
*   stxslus, enxslus, onto stretch of water body from .. m (stxslus)
*   to .. m (enxslus)
*
  tslus          mslus          stxslus          enxslus
      0.              0.001              20.                 320.
!  d             g/m^2           m                m              unit
! 0 ... 500.0  0 ... 1000.0      0 .... 10,000.                  range
*
*----END OF FILE---------------------------------------------------------------
```

Fig. 10 Example of a SL.INP file

Note that TOXSWA 1.2 simulates only user-specified data on spray drift. The drainage and runoff options are dummy values in TOXSWA 1.2. The next version of TOXSWA will be able to simulate the entry routes drainage and runoff.

Section 2
The number of loadings has to be entered. For each loading, the time of loading, the mass of the loading (in g m^{-2} water surface area) and start and end of the stretch of the water body over which the mass enters have to be given. The loadings should be entered in chronological order.

4.6 Substance: SU.INP

SU.INP contains data on the properties of the pesticide. An example of SU.INP is shown in Figure 11.

Section 1
The rate coefficient for transformation in the water layer (k) can be transformed into the half-life via $k = \ln(2) / DT_{50}$.

Section 2
The slope of the Freundlich-type isotherm for sorption to suspended solids based on the organic matter content ($K_{om,ss}$), the reference concentration at which the slope of the isotherm has been observed (c_e) and the Freundlich exponent for sorption to suspended solids (n_{ss}) have to be entered.

Section 3
The slope of the linear isotherm for sorption of the pesticide to macrophytes (K_{mp}) has to be entered.

Section 4
The exchange coefficients of the pesticide in water (k_l) and in air (k_g), the saturated vapour pressure (P), and the molecular mass of the pesticide (M) have to be entered. The temperatures indicate the temperature at which the saturated vapour pressure of the pesticide and the solubility of the pesticide in water were observed. These temperatures are used to calculate the proper Henry coefficient in TOXSWA.

Section 5
The diffusion coefficient of the pesticide in water (D_w) has to be entered.

Section 6
The rate coefficient for transformation in the sediment (k_b) can be transformed into to the half-life via: $k_b = \ln(2) / DT_{50}$.

Section 7
The slope of the Freundlich-type isotherm for sorption to sediment, based on the organic matter content ($K_{om,wb}$), the reference concentration at which the slope of the isotherm has been observed ($c_{e,wb}$) and the Freundlich exponent for sorption to sediment (n_{wb}) have to be entered.

```
*
*   TOXSWA input file
*   GUI version: 1.0
*
*   Filename: C:\TOXSWA\PESTICIDES\Cpf\SU.INP
*   Contents: Input data for TOXSWA concerning the substance
*   Date    : 2/22/99
*
*-----------------------------------------------------------------------------
*
*   Section 1: Transformation in water layer
*-----------------------------------------------------------------------------
*
*   half-life for transformation in water at 293 K
  dt50wl = 75.3                 ! unit: d         range: 0. .... 10000.
*   molar Arrhenius activation energy for transformation rate
*   (also used for sediment) (default value)
  aetf = 55000.                 ! unit: J/mol     range: 0. .... 1000000.
*
*-----------------------------------------------------------------------------
*
*   Section 2: Sorption suspended solids
*-----------------------------------------------------------------------------
*
*   slope sorption isotherm based at organic matter content, K_om,ss,
*   (distribution coefficient)
  kdomssdit = 16.4              ! unit: m^3/kg    range: 0. .... 1000.
*   concentration pesticide at which the K_om of the suspended solids
*   has been observed, c_e,ss (default value)
  coobkomss = 1.E-6             ! unit: kg/m^3    range: 1.E-6 .... 0.1
*   Freundlich exponent for sorption to suspended solids, n_ss
  exfrss = 0.9                  ! unit: -         range: 0.1 .... 2.
*
*-----------------------------------------------------------------------------
*
*   Section 3: Sorption to macrophytes
*-----------------------------------------------------------------------------
*
*   slope sorption isotherm based at dry weight macrophytes, K_mp
*   (distribution coefficient)
  kdmpdit = 0.                  ! unit: m^3/kg    range: 0. .... 1000.
*
*-----------------------------------------------------------------------------
*
*   Section 4: Volatilisation
*-----------------------------------------------------------------------------
*
*   molecular mass pesticide, M
  mamol = 350.6                 ! unit: g/mol     range: 10. .... 10000.
*   transport coefficient pesticide in liquid phase, k_l
  klq = 1.7                     ! unit: m/d       range: 0.1 .... 5.
*   transport coefficient pesticide in gas phase, k_g
  kga = 163.1                   ! unit: m/d       range: 0.1 .... 500.
*   saturated vapour pressure pesticide, P
  psat = 0.0025                 ! unit: Pa        range: 1E-15 .... 5000.
*   temperature at which saturated vapour pressure measured
  tepsat = 293.                 ! unit: K         range: 273. .... 373.
*   molar enthalpy of vaporisation (default value)
  mepsat = 95000.               ! unit: J/mol     range: 0. .... 1000000.
*   solubility pesticide in water, c_sol
  cosol = 2.                    ! unit: g/m^3     range: 1.E-6 .... 2000000.
*   temperature at which solubility is measured
  tesol = 293.                  ! unit: K         range: 273. .... 373.
*   molar enthalpy of dissolution (default value)
  mesol = 27000.                ! unit: J/mol     range: 0. .... 1000000.
*
```

Fig. 11 Example of a SU.INP file

```
*
+-------------------------------------------------------------------------------
*
*   Section 5: Exchange water column - sediment
+-------------------------------------------------------------------------------
*
*   diffusion coefficient pesticide in water, D_w (default value
  kdfw = 40.                    ! unit: mm^2/d     range: 1. .... 200.
*
+-------------------------------------------------------------------------------
*
*   Section 6: Transformation in sediment
+-------------------------------------------------------------------------------
*
*   half-life transformation sediment at 293 K
  dt50wb = 180.                 ! unit: d          range: 0. .... 10000.
*
+-------------------------------------------------------------------------------
*
*   Section 7: Sorption sediment
+-------------------------------------------------------------------------------
*
*   slope sorption isotherm based at organic matter content of
*   sediment material, K_om,wb, (distribution coefficient)
  kdomwbl = 16.4                ! unit: m^3/kg     range: 0. .... 1000.
*   concentration pesticide at which the K_om of the sediment material
*   has been observed, c_e,wb (default value)
  coobkomwb = 1.E-6             ! unit: kg/m^3     range: 1.E-6 .... 0.1
*   Freundlich exponent for sorption to sediment material, n_wb
  exfrwb = 0.9                  ! unit: -          range: 0.1 .... 2.
*
+----END OF FILE------------------------------------------------------------
```

(continuation of Fig. 11)

4.7 Input and output options

4.7.1 FILES.INP

This file gives the names of all of the input files, *including* their path (see Fig. 12).

```
*
*   TOXSWA input file
*   GUI version: 1.0
*   TOXSWA version: 1.2
*
*   Filename: C:\TOXSWA\RUNS\NLStandard_sp+Cpf\FILES.INP
*   Contents: Names of inputfiles for TOXSWA simulation
*   Date    : 4/13/99
*
*-------------------------------------------------------------------------------
*
*   Section 1: Path and names input files
*-------------------------------------------------------------------------------
*
  opoutinp = 'C:\TOXSWA\SCENARIOS\NLStandard_sp\OPOUT.INP' ! Output options
  wlnuinp = 'C:\TOXSWA\SCENARIOS\NLStandard_sp\WLNU.INP' ! Numerical
solution, time and length water body
  wlpainp = 'C:\TOXSWA\SCENARIOS\NLStandard_sp\WLPA.INP' ! Geometry and
other characteristics water body
  wlstinp = 'C:\TOXSWA\SCENARIOS\NLStandard_sp\WLST.INP' ! Initial
concentrations water layer
  wbnuinp = 'C:\TOXSWA\SCENARIOS\NLStandard_sp\WBNU.INP' ! Numerical
solution and thickness sediment
  wbpainp = 'C:\TOXSWA\SCENARIOS\NLStandard_sp\WBPA.INP' ! Characteristics
sediment
  wbstinp = 'C:\TOXSWA\SCENARIOS\NLStandard_sp\WBST.INP' ! Initial
concentrations sediment
  hyinp = 'C:\TOXSWA\SCENARIOS\NLStandard_sp\HY.INP' ! Hydrological
characteristics
  suinp = 'C:\TOXSWA\PESTICIDES\Cpf\SU.INP' ! Substance properties
  slinp = 'C:\TOXSWA\SCENARIOS\NLStandard_sp\SL.INP' ! Substance loadings
*
*----END OF FILE--------------------------------------------------------------
```

Fig. 12 Example of a FILES.INP file

4.7.2 OPOUT.INP

This file contains all of the options for the output of TOXSWA (see Fig. 13).

Section 1
The output files desired have to be selected in this section.

Section 2
The time step for output has to be entered.

Section 3
The number of sediment subsystems for which output is desired and the segment number of the water layer under which output of the sediment subsystems is desired have to be entered. Finally, the number of upper segments of the sediment, called the top layer, for which the pesticide mass will be accumulated and presented as output, has to be entered.

```
*   TOXSWA input file
*   GUI version: 1.0
*
*   Filename: C:\TOXSWA\SCENARIOS\NLStandard_sp\OPOUT.INP
*   Contents: Input data for TOXSWA concerning options for obtaining
*             model output
*   Date    : 2/10/99
*
*-------------------------------------------------------------------------------
*
*   Section 1: Selected output files
*-------------------------------------------------------------------------------
*
*   output file input.out (echo of all input) wanted? (0 = no, 1 = yes)
  op_input = 1                  ! unit: -         range: 0 .... 1
*   output file icwlhy.out (initial calculations for water layer and
*   hydrology) wanted? (0 = no, 1 = yes)
  op_icwlhy = 0                 ! unit: -         range: 0 .... 1
*   output file icwb.out (initial calculations for sediment) wanted?
*   (0 = no, 1 = yes)
  op_icwb = 0                   ! unit: -         range: 0 .... 1
*   output file wlmb.out (mass balance water layer) wanted? (0 = no,
*   1 = yes)
  op_wlmb = 1                   ! unit: -         range: 0 .... 1
*   output file wlmbsegmentnr.out (mass balance segment water layer)
*   wanted? (0 = no, 1 = yes)
  op_wlmbsegmentnr = 0          ! unit: -         range: 0 .... 1
*   output file wbsconondenr.out (concentrations sediment sub-system)
*   wanted? (0 = no, 1 = yes)
  op_wbscosegmentnr = 1         ! unit: -         range: 0 .... 1
*   output file wbmbsegmentnr.out (mass balance sediment sub-system)
*   wanted? (0 = no, 1 = yes)
  op_wbmbsegmentnr = 0          ! unit: -         range: 0 .... 1
*   output file wbmball.out (mass balance all sediment sub-systems)
*   wanted? (0 = no, 1 = yes)
  op_wbmball = 1                ! unit: -         range: 0 .... 1
*   output file dbsegmentnr.out (distribution substance in wl+wb at
*   segmentnr wl) wanted? (0 = no, 1 = yes)
  op_dbsegmentnr = 1            ! unit: -         range: 0 .... 1
*   output file dbdit.out (distribution substance in total water body)
*   wanted? (0 = no, 1 = yes)
  op_dbdit = 1                  ! unit: -         range: 0 .... 1
*   output file ecsegmentnr.out (exposure concentration at segmentnr)
*   wanted? (0 = no, 1 = yes)
  op_ecsegmentnr = 1            ! unit: -         range: 0 .... 1
*
*-------------------------------------------------------------------------------
*
*   Section 2: Timestep for output
*-------------------------------------------------------------------------------
*
*   timestep for output (should be a multiple of the selected calculation
*   timestep deltwl)
  deltout = 0.5                 ! unit: d         range: 0.001 .... 25.
*
*-------------------------------------------------------------------------------
*
*   Section 3: Selected segments wl + sediment sub-systems for output
*-------------------------------------------------------------------------------
*
*   number of segments wl, coupled to sediment sub-systems, for which
*   output is wanted (max. of 9)
  nwbsy = 5                     ! unit: -         range: 0 .... 9
*   segment number in water layer at/or under which output is wanted
  iwbsy =  1     ! unit: -       range: 1 .... 200
           20 40 60 80
*   number of upper segments forming the top layer for which the
*   accumulated pesticide mass will be calculated
  ktop = 7                      ! unit: -         range: 1 .... 100
*
*---END OF FILE---------------------------------------------------------------
```

Fig. 13 Example of an OPOUT.INP file

5 Description of output files

5.1 Introduction

The program produces a minimum of two and a maximum of 53 output files, depending on the number of segments of the water layer and the underlying sediment subsystems for which local output is desired. Output at specific locations in the water body is optional. The water layer segments and underlying sediment subsystems for which output is desired are entered in OPOUT.INP. The TOXSWA program automatically adjusts the names of the output files to the water layer segment numbers. The output files are:

INPUT.OUT	reproduction of input
ICWLHY.OUT	water layer plus hydrology; calculations defining initial conditions
ICWB.OUT	sediment; calculations defining initial conditions
MESSAGE.OUT	warning and error messages
WLSOCO.OUT	water layer; concentrations, lineic mass, distribution
WBSCOxxx.OUT	sediment / subsystem xxx; concentrations, lineic mass, distribution
WLMB.OUT	water layer; mass balance for entire water body
WLMBxxx.OUT	water layer / segment xxx; mass balance
WBMBALL.OUT	sediment; mass balance under entire length of water body
WBMBxxx.OUT	sediment / subsystem xxx; mass balance
DBDIT.OUT	water body: momentary distribution between compartments
DBxxx.OUT	water body / segment xxx: momentary distribution between compartments
ECxxx.OUT	water layer and sediment / segment xxx exposure concentrations

The contents of the output files are described in more detail in the Sections 5.2 to 5.5.

Several output files present mass balances. If the percentage of the mass that is missing exceeds 0.1% a warning is given in MESSAGE.OUT. It should be checked whether errors have been made, or whether the missing mass is due to a normal accumulation of small errors caused by the numerical solution of the mass conservation equations (i.e. building up after many time steps). Results with a poor mass balance indicate than there is something wrong.

The output files are briefly described below, with an example of each of the files. The presented output files belong to the example simulation shown in Chapter 3.

Some of the output files were too large to show completely in this manual. If results are given for e.g. many time steps, only some first time steps are shown, followed by a dot.

5.2 Input, initial conditions and messages

5.2.1 INPUT.OUT

This file reproduces the input of the input files and the values set for each of the segments (see Fig. 14).

```
TOXSWA simulation:  22- 2-1999  14:49:24
Output of input:


Simulation with TOXSWA version: 1.2.1


All input from subroutine opout:

Input from C:\TOXSWA\RUNS\NLStandard_sp+Example_pesticide\FILES.INP :
Section 1: Filenames inputfiles
C:\TOXSWA\SCENARIOS\NLStandard_sp\OPOUT.INP
C:\TOXSWA\SCENARIOS\NLStandard_sp\WLNU.INP
C:\TOXSWA\SCENARIOS\NLStandard_sp\WLPA.INP
C:\TOXSWA\SCENARIOS\NLStandard_sp\WLST.INP
C:\TOXSWA\SCENARIOS\NLStandard_sp\WBNU.INP
C:\TOXSWA\SCENARIOS\NLStandard_sp\WBPA.INP
C:\TOXSWA\SCENARIOS\NLStandard_sp\WBST.INP
C:\TOXSWA\SCENARIOS\NLStandard_sp\HY.INP
C:\TOXSWA\PESTICIDES\Cpf\SO.INP
C:\TOXSWA\SCENARIOS\NLStandard_sp\SL.INP


Input from C:\TOXSWA\SCENARIOS\NLStandard_sp\OPOUT.INP  :
Section 1: Selected output files:       (no dimensions)
          1
          0
          0
          1
          0
          1
          0
          1
          1
          1
          1
Section 2: Timestep for output (d):
   5.000000E-01
Section 3: Selected sediment subsystems for output:   (no dimensions)
          5
          1          20          40          60          80
          7

All input data from wlin:

Input from C:\TOXSWA\SCENARIOS\NLStandard_sp\WLNU.INP :
Section 1: Numerical weight factors   (no dimensions)
   5.000000E-01        1.000000
Section 2: Time parameters    (s, resp d)
    3600.000000       20.000000
Section 3: Space parameters     (m)
     320.000000    0.000000E+00    0.000000E+00
Section 4: Number segments   (no dimensions)
        80           0           0
```

Fig 14 Example of an INPUT.OUT file

```
Section 5: Lengths segments      (m)

        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000


 Input from C:\TOXSWA\SCENARIOS\NLStandard_sp\WLPA.INP
:
 Section 1: geometry ditch    (m, dimensionless, resp m)
   4.000000E-01       1.000000    1.000000E-01
 Section 2: Geometry neighbouring plot      (m)
     999.000000
 Section 3: Concentration and org. matter susp.solids    (g/m^3, dimensionless
      15.000000    5.000000E-01
 Section 4: Amount macrophytes     (g/m^2
    0.000000E+00

 Input from C:\TOXSWA\SCENARIOS\NLStandard_sp\WLST.INP
:
 Section 1: Initial concentrations (g/m^3)
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
 section 3: Background concentration     (g/m^3)
    0.000000E+00


 All input data from wbin:

 Input from C:\TOXSWA\SCENARIOS\NLStandard_sp\WBNU.INP :
 Section 1: Numerical weight factors    (no dimensions)
    5.000000E-01       1.000000
 Section 2: Time parameters         (s)
     3600.000000
 Section 3: Space parameters         (m)
    1.000000E-01    0.000000E+00
```

(continuation of Fig 14)

```
 Section 4: Number segments   (no dimensions)
          14             0
  Section 5: Lengths segments          (m)
     1.000000E-03    1.000000E-03    1.000000E-03    1.000000E-03
     2.000000E-03    2.000000E-03    2.000000E-03    5.000000E-03
     5.000000E-03    1.000000E-02    1.000000E-02    2.000000E-02
     2.000000E-02    2.000000E-02


  Input from C:\TOXSWA\SCENARIOS\NLStandard_sp\WBPA.INP
:
  Section 1: Physical properties sediment   (kg/m^3, (2x) dimensionless)
        80.000000       80.000000       80.000000       80.000000
        80.000000       80.000000       80.000000      220.000000
       220.000000      670.000000      670.000000     1500.000000
      1500.000000     1500.000000
     8.200000E-01    8.200000E-01    8.200000E-01    8.200000E-01
     8.200000E-01    8.200000E-01    8.200000E-01    7.700000E-01
     7.700000E-01    6.200000E-01    6.200000E-01    3.600000E-01
     3.600000E-01    3.600000E-01
     8.200000E-01    8.200000E-01    8.200000E-01    8.200000E-01
     8.200000E-01    8.200000E-01    8.200000E-01    7.700000E-01
     7.700000E-01    6.200000E-01    6.200000E-01    2.800000E-01
     2.800000E-01    2.800000E-01
  Section 2: Organic matter sediment   (dimensionless)
     2.500000E-01    2.500000E-01    2.500000E-01    2.500000E-01
     2.500000E-01    2.500000E-01    2.500000E-01    1.900000E-01
     1.900000E-01    6.000000E-02    6.000000E-02    2.000000E-02
     2.000000E-02    2.000000E-02
  Section 3: Dispersion length          (m)
     1.500000E-02

  Input from C:\TOXSWA\SCENARIOS\NLStandard_sp\WBST.INP
:
  Section 1: Initial concentrations   (g/m^3
     0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
     0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
     0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
     0.000000E+00    0.000000E+00


  All input from subroutine hyin:

  Input from C:\TOXSWA\SCENARIOS\NLStandard_sp\HY.INP
:
  Section 1: Flow velocity and water depth   (m/d, resp m)
       10.000000     3.000000E-01
  Section 2: Dispersion coefficient      (m^2/d)
       20.000000

  Section 3: Seepage with concentration   (m^3/m^2.d, resp g/m^3)
     0.000000E+00    0.000000E+00

  Section 4: Temperature (K)
      283.000000
```

(continuation of Fig 14)

```
All input from subroutine suin:

Input from C:\TOXSWA\PESTICIDES\Cpf\SU.INP:

Section 1: Transformation in water layer   (d)     (J/mol)
      75.300000     55000.000000
section 2: Sorption susp. solids   (m^3/kg, kg/m^3, resp. dimensionless)
      16.400000     1.000000E-06     9.000000E-01
Section 3: Sorption to macrophytes   (m^3/kg)
    0.000000E+00
Section 4: Volatilisation   (g/mol, m/d, m/d, Pa, K, J/mol, g/m^3, K, J/mol)
     350.600000        1.700000      163.100000
   2.500000E-03      293.000000    95000.000000
      2.000000      293.000000    27000.000000
Section 5: Exchange water layer - sed.   (mm^2/d)
      40.000000
Section 6: Transformation in sediment    (d)
     180.000000
Section 7: Sorption sediment   (m^3/kg, kg/m^3, resp. dimensionless)
      16.400000     1.000000E-06     9.000000E-01


All input from subroutine slin:

Input from C:\TOXSWA\SCENARIOS\NLStandard_sp\SL.INP
:
Section 1: Options data sources, entry routes
 User specified, spray drift:          1
 User specified, drainage   :          0
 User specified, runoff     :          0
 Model output, drainage     :          0
 Model output, runoff       :          0

Section 2: User specified input, spray drift
number of loadings
-
time, mass and stretch of watercourse
(d, g/m^2, m, m)
          1
   0.000000E+00    1.000000E-03       20.000000       320.000000
```

(continuation of Fig 14)

5.2.2 ICWLHY.OUT

This file presents the results of the calculations executed to define the initial situation in the water layer and the hydrology. Figure 15 shows an example.

```
 TOXSWA simulation:  15- 3-1999   9:39:10
 Output of initial calculations water layer and hydrology:

 Results from subroutine hyin:
 discharge equals    .2431E-04 m3.s-1

 Results of some initial calculations from subroutine suin:
 kdfrss(1-nxnotot)    (m^3/kg)
    8.200000E-03    8.200000E-03    8.200000E-03    8.200000E-03
    8.200000E-03    8.200000E-03    8.200000E-03    8.200000E-03
    8.200000E-03    8.200000E-03    8.200000E-03    8.200000E-03
.
.

 Results of initial calculations from subroutine wlit:
 delx(1-nxnotot):   (m)
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
        4.000000        4.000000        4.000000        4.000000
.
.

4.000000        4.000000        4.000000        4.000000
 xcd(1-nxnotot):   (m)
        2.000000        6.000000       10.000000       14.000000
       18.000000       22.000000       26.000000       30.000000
       34.000000       38.000000       42.000000       46.000000
.
.

 Results of calculations from subroutine wlitnu:
 num. weight factors for all segments:
  segmentnumber    nwwmh          nwwph          (dimensionless)
              1    0.000000E+00    5.000000E-01
              2    5.000000E-01    5.000000E-01
              3    5.000000E-01    5.000000E-01
.
.

Results of calculations from subroutine wlitco:
 length exchanging perimeter, pez0hw:   (m)
    6.828427E-01
 initial wetted area ditch for all segments, warst(1-nxnotot):   (m2)
    2.100000E-01    2.100000E-01    2.100000E-01    2.100000E-01
    2.100000E-01    2.100000E-01    2.100000E-01    2.100000E-01
    2.100000E-01    2.100000E-01    2.100000E-01    2.100000E-01
.
.
```

Fig. 15 Example of ICWLHY.OUT

```
initial concentrations for all segments
 segmentnr, total, dissolved, at macrophytes and at susp solids
     ixnotot     castwl(i)        co(i)          somp(i)  and   soss(i)
                 (g.(m)-3        g.(m)-3         g.(g)-1        g.(g)-1)
           1    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
           2    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
           3    0.000000E+00    0.000000E+00    0.000000E+00    0.000000E+00
.
.

 Results of calculations from subroutine wlsoge (for first timestep):
 first water depth at interfaces for all segments:
    ixnotot     wdhjimh         wdhjiph        (m)
 then wetted area at interfaces at time j+1/2 for all segments:
                 warjphimh       warjphiph     (m2)

    ixnotot     wdhjimh         wdhjiph        (m)
                warjphimh       warjphiph     (m2)
           1    3.000000E-01     3.000000E-01
                .2100000         .2100000

    ixnotot     wdhjimh         wdhjiph        (m)
                warjphimh       warjphiph     (m2)
           2    3.000000E-01     3.000000E-01
                .2100000         .2100000

    ixnotot     wdhjimh         wdhjiph        (m)
                warjphimh       warjphiph     (m2)
           3    3.000000E-01     3.000000E-01
                .2100000         .2100000
.
.

 Some calculation results from subroutine wlsods:
 physical, numerical and calculation dispersion for
 first timestep and first segment
 kds  kdswnujiph  kdswcljiph  (m2.(day)-1)
      20.000000       -2.083333       22.083330


 Results from subroutine wlso

 positivity conditions are: lbd =< 0     rbd >= 0
                            ldd > 0      rdd > 0
                            lod =< 0     rod >= 0

 lbd     rbd     timestep   segmentnumber
 ldd     rdd
 lod     rod
    rv
    0.000000E+00    2.334954E-02          1          1
       4.303784        3.802137
    0.000000E+00    0.000000E+00
    0.000000E+00

 lbd     rbd     timestep   segmentnumber
 ldd     rdd
 lod     rod
    rv
    0.000000E+00    2.334954E-02          1          2
       4.303784        3.778787
    0.000000E+00    4.716604E-01
    0.000000E+00
.
.
```

(continuation of Fig 15)

5.2.3 ICWB.OUT

This file presents the results of the calculations executed to define the initial situation in the sediment. Figure 16 shows an example.

```
 TOXSWA simulation:  15- 3-1999   9:39:10
 Results from initial calculations for sediment:


 Results of some initial calculations from subroutine suin:
 kdfrwb(1-nznotot):   (m^3/kg)
    4.100000E-03    4.100000E-03    4.100000E-03    4.100000E-03
    4.100000E-03    4.100000E-03    4.100000E-03    3.116000E-03
    3.116000E-03    9.839999E-04    9.839999E-04    3.280000E-04
    3.280000E-04    3.280000E-04

 Results of initial calculations from subroutine wbit:
 delz(1-nznotot) from wbit:   (m)
    1.000000E-03    1.000000E-03    1.000000E-03    1.000000E-03
    2.000000E-03    2.000000E-03    2.000000E-03    5.000000E-03
    5.000000E-03    1.000000E-02    1.000000E-02    2.000000E-02
    2.000000E-02    2.000000E-02
 zcd(1-nznotot) from wbit:   (m)
    5.000000E-04    1.500000E-03    2.500000E-03    3.500000E-03
    5.000000E-03    7.000000E-03    9.000001E-03    1.250000E-02
    1.750000E-02    2.500000E-02    3.500000E-02    5.000000E-02
    7.000000E-02    9.000000E-02

 Results of initial calculations from subroutine wbitnu:
 num. weight factors for all segments:
  segment number     nwbmh           nwbph       (dimensionless)
             1    0.000000E+00    5.000000E-01
             2    5.000000E-01    5.000001E-01
             3    5.000001E-01    4.999999E-01
.
.

 Results of initial calculations from subroutine wbitge:
 length perimeter at segments and interfaces for all segments:
  segment number      pemh            pe             peph          (m)
             1    6.828427E-01    6.846712E-01    6.864996E-01
             2    6.864996E-01    6.883280E-01    6.901565E-01
             3    6.901565E-01    6.919848E-01    6.938133E-01
.
.

porosity at interfaces for all segments:
  segment number     pormh           porph       (dimensionless)
             1    8.200000E-01    8.200000E-01
             2    8.200000E-01    8.200000E-01
             3    8.200000E-01    8.200000E-01.
.

bulkdensity at interfaces for all segments:
  segment number    bdwbmh          bdwbph      (g.(m)-3)
             1    80000.000000    80000.000000
             2    80000.000000    80000.000000
             3    80000.000000    80000.000000
.
.
```

Fig. 16 Example of an ICWB.OUT file

```
 Freundlich sorption coefficient at interfaces for all segments:
 Segment number    kdfrwbmh        kdfrwbph     (m3.(g)-1)
          1    4.100000E-03    4.100000E-03
          2    4.100000E-03    4.100000E-03
          3    4.100000E-03    4.100000E-03
.
.

diffusion coefficients at interfaces for all segments:
 segment number    kdfwbmh         kdfwbph      (m3.(g)-1)
          1    3.796296E-10    3.796296E-10
          2    3.796296E-10    3.796296E-10
          3    3.796296E-10    3.796296E-10
.
.

 Results of initial calculations from subroutine wbitco:
 initial concentrations for all segments
       segment nr,  total,          dissolved and  sorbed at solid bottom mat.
     kznotot    castwb(k)       co(k)          sowb(k)
                (g.(m)-3        g.(m)-3        g.(g)-1)
          1    0.000000E+00    0.000000E+00    0.000000E+00
          2    0.000000E+00    0.000000E+00    0.000000E+00
          3    0.000000E+00    0.000000E+00    0.000000E+00
.
.

 Some calculation results from subroutine wbsods:
 physical, numerical and calculation dispersion for first timestep and
 first segment sediment under first segment water layer
  kdswbjph(k)  kdsbnujkph(k)   kdsbcijkph(k)  (m2.(day)-1)
    0.000000E+00    0.000000E+00    0.000000E+00

 Results from subroutine wbso

 positivity conditions are: blbd =< 0    brbd >= 0
                            bldd > 0     brdd > 0
                            blod =< 0    brod >= 0

 blbd    brbd    time step   segment number
 bldd    brdd
 blod    brod
    brv
    0.000000E+00       1.123659          1          1
    51985.380000    51978.260000
    0.000000E+00    0.000000E+00
    2.235348E-25

 blbd    brbd    time step   segment number
 bldd    brdd
 blod    brod
    brv
    0.000000E+00       1.123643          1          2
    51985.380000    51979.380000
    0.000000E+00       1.117690
    0.000000E+00

 blbd    brbd    time step   segment number
 bldd    brdd
 blod    brod
.
```

(continuation of Fig. 16)

5.2.4 MESSAGE.OUT

This file repeats all the warning and error messages, which have been directed to the screen during execution (see Fig. 17). Some messages of the TTUTIL package, used for input range checking and for opening and deleting temporary files, are given at the top of the MESSAGE.OUT file. If a message concerning the mass balance is given over 20 times, or a message concerning the positivity conditions is given over 50 times, it is no longer written to MESSAGE.OUT, in order to prevent the file becoming extremely large. All possible warning and error messages have been explained in Annex 2.

```
 TOXSWA simulation:  15- 3-1999   9:39:10
 Messages (error/warning/ttutil):

 Data file   DE\FILES.INP with  10 variables parsed by RDINDX
 Data file   SP\OPOUT.INP with  15 variables parsed by RDINDX
 Data file   _SP\WLNU.INP with  13 variables parsed by RDINDX
 Data file   _SP\WLPA.INP with   7 variables parsed by RDINDX
 Data file   _SP\WLST.INP with   2 variables parsed by RDINDX
 Data file   _SP\WBNU.INP with   9 variables parsed by RDINDX
 Data file   _SP\WBPA.INP with   5 variables parsed by RDINDX
 Data file   _SP\WBST.INP with   1 variables parsed by RDINDX
 Data file   RD_SP\HY.INP with   6 variables parsed by RDINDX
 Data file   ICIDE\SU.INP with  20 variables parsed by RDINDX
 Data file   RD_SP\SL.INP with  10 variables parsed by RDINDX

 Temporary file C:\TOXSWA\RUNS\NLSTANDARD_SP+EXAMPLE_PESTICIDE\FILES.TMP
deleted by RDDTMP
 Temporary file C:\TOXSWA\SCENARIOS\NLSTANDARD_SP\OPOUT.TMP deleted by RDDTMP
 Temporary file C:\TOXSWA\SCENARIOS\NLSTANDARD_SP\WLNU.TMP deleted by RDDTMP
 Temporary file C:\TOXSWA\SCENARIOS\NLSTANDARD_SP\WLPA.TMP deleted by RDDTMP
 Temporary file C:\TOXSWA\SCENARIOS\NLSTANDARD_SP\WLST.TMP deleted by RDDTMP
 Temporary file C:\TOXSWA\SCENARIOS\NLSTANDARD_SP\WBNU.TMP deleted by RDDTMP
 Temporary file C:\TOXSWA\SCENARIOS\NLSTANDARD_SP\WBPA.TMP deleted by RDDTMP
 Temporary file C:\TOXSWA\SCENARIOS\NLSTANDARD_SP\WBST.TMP deleted by RDDTMP
 Temporary file C:\TOXSWA\SCENARIOS\NLSTANDARD_SP\HY.TMP deleted by RDDTMP
 Temporary file C:\TOXSWA\PESTICIDES\EXAMPLE_PESTICIDE\SU.TMP deleted by
RDDTMP
 Temporary file C:\TOXSWA\SCENARIOS\NLSTANDARD_SP\SL.TMP deleted by RDDTMP
```

Fig. 17 Example of a MESSAGE.OUT file

5.3 Mass balances

5.3.1 WLMB.OUT

This file contains the mass balance of the water layer calculated at selected time steps of output. The mass balance is a useful tool to check whether the mass introduced into the system has not disappeared because of a numerical artefact of the model. Figure 18 shows an example of WLMB.OUT. The masses introduced into the system are the positive terms of the mass balance, the total mass in the water layer at the start of the simulation plus the loadings during the simulation (column 2), plus the cumulative input coming in via the sediment (column 3). The negative terms of the mass balance are the total mass in the water layer at the

```
.* Output of mass balance of the entire water layer
 * as a function of time
 *
 * Mass balance, percentage of initial, loaded and incoming mass from the sediment
 *
 *<====>  <= positive terms ===>  <= negative terms=====================================================>  <====================>  <====>
 *  time init.+load.  from sed.   remaining   to sedim.     volatil.     transf.      out end   out front      balance      balance  timest
 *     d          g           g           g           g           g           g           g           g            g            %
 *
   0.000  0.3000E+00  0.0000E+00  0.3000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  -.2921E-05  -.9735E-03      0
   0.500  0.3000E+00  0.0000E+00  0.2662E+00  -.2161E-01  -.6848E-02  -.5863E-03  -.4753E-02  0.0000E+00  -.2797E-05  -.9323E-03     72
   1.000  0.3000E+00  0.0000E+00  0.2376E+00  -.3926E-01  -.1293E-01  -.1108E-02  -.9055E-02  0.0000E+00  -.3017E-05  -.1006E-02    144
   1.500  0.3000E+00  0.2135E-05  0.2135E+00  -.5359E-01  -.1838E-01  -.1575E-02  -.1297E-01  0.0000E+00  -.2825E-05  -.9416E-03    216
   2.000  0.3000E+00  0.1832E-04  0.1930E+00  -.6519E-01  -.2328E-01  -.1996E-02  -.1656E-01  0.0000E+00  -.2834E-05  -.9445E-03    288
   2.500  0.3000E+00  0.6195E-04  0.1755E+00  -.7459E-01  -.2772E-01  -.2378E-02  -.1988E-01  0.0000E+00  -.3038E-05  -.1012E-02    360
   3.000  0.3000E+00  0.1421E-03  0.1605E+00  -.8221E-01  -.3177E-01  -.2726E-02  -.2295E-01  0.0000E+00  -.2933E-05  -.9773E-03    432
 .
 .
  30.000  0.3000E+00  0.2761E-01  0.1578E-01  -.1155E+00  -.9821E-01  -.8494E-02  -.8963E-01  0.0000E+00  -.3179E-05  -.9702E-03   4320
```

Fig. 18 Example of a WLMB.OUT file

time when the mass balance is calculated (column 4), the cumulative mass that has penetrated into the sediment since the start of the simulation (column 5), the cumulative mass that has volatilised to the air (column 6), the cumulative mass that has been transformed (column 7), the cumulative mass that has flowed out of the water body at the downstream end of the water body (column 8) and the cumulative mass that was transported across the upstream boundary of the water body (column 9).

The quantity missing from the water layer of the water body, which is the sum of the positive and negative terms of the balance is given in grams in column 10 and in percentage of the total mass that has entered the water body in the period between the start of the simulation and the time of output (the positive terms) in column 11.

5.3.2 WLMBxxx.OUT

This file shows the mass balance per running metre of the water body in the water layer located in the segment xxx (see Fig. 19). The file is equivalent to WLMB.OUT. The masses introduced into the segment are the positive terms of the mass balance, the total mass in the water layer segment at the start of the simulation plus the loadings during the simulation (column 2), the cumulative input from the segment upstream of the segment considered (column 3), the cumulative input from then segment downstream of the segment considered (column 4) and the cumulative input via the sediment (column 5). The negative terms of the mass balance are the total mass in the segment at the time when the mass balance is calculated (column 6), the cumulative mass that was transported to the segment upstream of the segment considered (column 7), the cumulative mass flowed out to the segment downstream the segment considered (column 8), the cumulative mass that has penetrated into the sediment (column 9), the cumulative mass that has volatilised to the air (column 10) and the cumulative mass that has been transformed (column 11).

The quantity missing from the water layer segment, which is the sum of the positive and negative terms of the balance is given in grams in column 12, and in percentage of the total mass that has entered the segment of the water body in the period between the start of the simulation and the time of output (the positive terms), in column 13.

```
* Output of mass balance of segment  80 of the
* water layer as a function of time (middle of segment is at   318.000 m)
*
* Mass balance per running metre of the water body
* percentage of initial, loaded and incoming mass from the sediment
*
*<===>  <= positive terms ========================> <= negative terms===============================================> <===================> <===>
*  time init.+load.   in front     in end   from sed.  remaining    out end  out front    to  sed.   volatil.     transf.     balance    balance timest
*     d     g.m'-1     g.m'-1     g.m'-1     g.m'-1     g.m'-1     g.m'-1     g.m'-1     g.m'-1     g.m'-1      g.m'-1      g.m'-1          %
*
  0.000 0.1000E-02 0.0000E+00 0.0000E+00 0.0000E+00 0.1000E-02 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 -.9197E-08 -.9197E-03      0
  0.500 0.1000E-02 0.1188E-02 0.0000E+00 0.0000E+00 0.9024E-03 -.1188E-02 0.0000E+00 -.7262E-04 -.2301E-04 -.1970E-05 -.8866E-08 -.4052E-03     72
  1.000 0.1000E-02 0.2264E-02 0.0000E+00 0.0000E+00 0.8194E-03 -.2264E-02 0.0000E+00 -.1330E-03 -.4382E-04 -.3753E-05 -.9035E-08 -.2768E-03    144
  1.500 0.1000E-02 0.3243E-02 0.0000E+00 0.0000E+00 0.7488E-03 -.3243E-02 0.0000E+00 -.1831E-03 -.6276E-04 -.5378E-05 -.9075E-08 -.2139E-03    216
  2.000 0.1000E-02 0.4141E-02 0.0000E+00 0.0000E+00 0.6885E-03 -.4141E-02 0.0000E+00 -.2245E-03 -.8010E-04 -.6867E-05 -.9346E-08 -.1818E-03    288
  2.500 0.1000E-02 0.4969E-02 0.0000E+00 0.0000E+00 0.6369E-03 -.4969E-02 0.0000E+00 -.2588E-03 -.9608E-04 -.8239E-05 -.9276E-08 -.1554E-03    360
  3.000 0.1000E-02 0.5737E-02 0.0000E+00 0.0000E+00 0.5923E-03 -.5737E-02 0.0000E+00 -.2873E-03 -.1109E-03 -.9513E-05 -.9533E-08 -.1415E-03    432
.
.
 30.000 0.1000E-02 0.2240E-01 0.0000E+00 0.2015E-04 0.1140E-03 -.2241E-01 0.0000E+00 -.4325E-03 -.4296E-03 -.3716E-04 -.1359E-07 -.5801E-04   4320
```

Fig. 19 Example of a WLMBxxx.OUT file

5.3.3 WBMBALL.OUT

This file contains the mass balance of the sediment under the entire water body for the time steps of output; it is the sum of the mass in all sediment subsystems. An example is shown in Figure 20. The positive terms of the mass balance are the total mass in the sediment at the start of the simulation (column 2), the cumulative mass that has entered the sediment from the water layer since the start of the simulation (column 3) and the cumulative mass that has entered the sediment via upward seepage (column 4). The negative terms of the mass balance are the total mass in the sediment at the time step for which the mass balance has been made up (column 5), the cumulative mass that has left the sediment by moving into the water layer (column 6), the cumulative mass that has percolated out of the sediment (column 7) and the cumulative mass that has been transformed since the start of the simulation (column 8). The missing quantity of mass for the sediment in all subsystems is given in column 9, which is the sum of all positive and negative terms. Column 10 indicates the percentage missing mass, calculated on the sum of the initial mass in the sediment plus the mass that has entered the sediment from the water layer and from below via upward seepage during the period simulated. Finally, column 11 gives the cumulative mass of substance in the selected number of upper segments, forming the top layer of the sediment.

5.3.4 WBMBxxx.OUT

This file shows the mass balance in the sediment subsystem under segment number xxx of the water layer (Fig. 21). The file is identical to WBMBALL.OUT, except that it concerns the masses in one sediment subsystem (xxx) only.

```
* Output of mass balance of the entire sediment (all sediment subsystems of water body)
* as a function of time
*
* Mass balance, percentage of initial and incoming mass (from water layer and upward seepage)
*
* Thickness of selected top layer is   10.00 mm
*
*<====>  <= positive terms ===============>  <= negative terms ===========================>  <====================>  <========>  <====>
*  time      initial      from wl      seepage    remaining        to wl   percolated       transf.      balance      balance   top layer  timest
*     d            g            g            g            g            g            g            g            g            %            g
*
  0.000  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00      0
  0.500  0.0000E+00  0.2161E-01  0.0000E+00  0.2159E-01  0.0000E+00  0.0000E+00  -.1717E-04  -.1812E-07  -.8387E-04  0.2159E-01     72
  1.000  0.0000E+00  0.3926E-01  0.0000E+00  0.3919E-01  0.0000E+00  0.0000E+00  -.6489E-04  0.1417E-06  0.3610E-03  0.3919E-01    144
  1.500  0.0000E+00  0.5359E-01  0.0000E+00  0.5345E-01  -.2135E-05  0.0000E+00  -.1374E-03  0.2568E-06  0.4793E-03  0.5345E-01    216
  2.000  0.0000E+00  0.6519E-01  0.0000E+00  0.6494E-01  -.1832E-04  0.0000E+00  -.2300E-03  0.3092E-06  0.4743E-03  0.6494E-01    288
  2.500  0.0000E+00  0.7459E-01  0.0000E+00  0.7419E-01  -.6195E-04  0.0000E+00  -.3387E-03  0.3715E-06  0.4980E-03  0.7419E-01    360
  3.000  0.0000E+00  0.8221E-01  0.0000E+00  0.8161E-01  -.1421E-03  0.0000E+00  -.4605E-03  0.5332E-06  0.6485E-03  0.8161E-01    432
.
.
 30.000  0.0000E+00  0.1155E+00  0.0000E+00  0.7940E-01  -.2761E-01  0.0000E+00  -.8494E-02  -.2274E-05  -.1969E-02  0.7940E-01   4320
```

Fig. 20 Example of a WBMBALL.OUT file

```
* Output of mass balance of the sediment subsystem under segment  80 of water layer
* as a function of time at  (middle of segment is at   318.000 m)
*
* Mass balance, percentage of initial and incoming mass (from water layer and upward seepage)
*
* Thickness of selected top layer is   10.00 mm
*
*<====>  <= positive terms ==============>  <= negative terms ============================>  <====================>  <========>  <====>
*  time      initial      from wl      seepage    remaining        to wl   percolated       transf.      balance      balance    top layer  timest
*     d      g.m'-1       g.m'-1       g.m'-1       g.m'-1       g.m'-1       g.m'-1        g.m'-1       g.m'-1            %       g.m'-1
*
  0.000  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00      0
  0.500  0.0000E+00  0.7262E-04  0.0000E+00  0.7257E-04  0.0000E+00  0.0000E+00  -.5755E-07  0.6430E-10  0.8854E-04  0.7257E-04     72
  1.000  0.0000E+00  0.1330E-03  0.0000E+00  0.1328E-03  0.0000E+00  0.0000E+00  -.2187E-06  0.3981E-09  0.2993E-03  0.1328E-03    144
  1.500  0.0000E+00  0.1831E-03  0.0000E+00  0.1826E-03  0.0000E+00  0.0000E+00  -.4655E-06  0.8785E-09  0.4798E-03  0.1826E-03    216
  2.000  0.0000E+00  0.2245E-03  0.0000E+00  0.2237E-03  0.0000E+00  0.0000E+00  -.7832E-06  0.1081E-08  0.4816E-03  0.2237E-03    288
  2.500  0.0000E+00  0.2588E-03  0.0000E+00  0.2577E-03  0.0000E+00  0.0000E+00  -.1159E-05  0.1429E-08  0.5521E-03  0.2577E-03    360
  3.000  0.0000E+00  0.2873E-03  0.0000E+00  0.2857E-03  0.0000E+00  0.0000E+00  -.1584E-05  0.1865E-08  0.6493E-03  0.2857E-03    432
.
.
 30.000  0.0000E+00  0.4325E-03  0.0000E+00  0.3774E-03  -.2015E-04  0.0000E+00  -.3495E-04  -.9131E-09  -.2111E-03  0.3774E-03   4320
```

Fig. 21 Example of a WBMBxxx.OUT file

5.4 Concentrations and distribution between the compartments

5.4.1 WLSOCO.OUT

This file presents the output of the calculations of subroutine WLSOCO.FOR (see Fig. 22). For each of the time steps for output (column 1), and each of the water layer segments (column 2), the concentrations of the substance in the water layer are given: total (column 4), dissolved (column 5), adsorbed to macrophytes (column 6) and adsorbed to suspended solids (column 7). The table also shows how the total mass present in the water layer is distributed between the three compartments (columns 8-11) mentioned above. The distributions are calculated from the lineic masses. Column 3 indicates at which distance in the water body the output is given (middle of segment indicated in column 2).

5.4.2 WBSCOxxx.OUT

This file shows the output of the calculations of subroutine WBSO.FOR (see Fig. 23). The file lists the segments of the sediment subsystem for each time step of output (column 1). The table presents for each segment of the subsystem (column 2, middle of segment indicated in column 3): total concentrations (column 4), dissolved (column 5) and adsorbed (column 5). The columns 7-9 indicate how the total mass present in sediment subsystem xxx is distributed between the dissolved and adsorbed phases.

In the rows indicated in the segment column (2) by ' top' the same output is given for the top layer of the sediment. The values are depth-weighed averages. The thickness of the top layer is indicated in the header of the file.

5.4.3 DBDIT.OUT

This file shows the distribution of the pesticide mass between compartments of the water layer and the sediment for the entire water body (see Fig. 24). For each time step, it shows, the total mass in the water layer (column 2) the mass dissolved in the water layer (column 3), the mass sorbed to the macrophytes (column 4), the mass sorbed to the suspended solids (column 5), the total mass in the sediment (column 6), the mass dissolved in the sediment (column 7), and the mass sorbed to the solid phase in the sediment (column 8). Next to this, the distribution between the water layer (column 9) and the sediment (column 10) is given in percentages of the total mass.

5.4.4 DBxxx.OUT

This file shows the distribution of the pesticide mass between all compartments of the water layer and the sediment at the location of segment xxx in the water layer (see Fig. 25). The content of the file is identical to that of DBDIT.OUT. It considers the lineic mass present in the water layer segment as well as the lineic mass present in the sediment subsystem below the specified segment in the water layer.

```
* Output of concentrations and distribution percentages
* as a function of time for all segments of the water layer
*
* Percentage of total present calculated from
* lineic mass (mass per running metre ditch)
*
*<====>  <=>  <=======>    <= concentrations =================================>    <= distribution water layer =>  <====>
*  time  segm  distance          total       dissolved    macrophytes    susp.solids     total dissol macroph susp.s.  timest
*                                   c*               c            Xmp            Xss
*     d                 m        g.m-3           g.m-3          g.g-1          g.g-1         %      %       %       %
*
  0.000     1     2.000    0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00      0.00   0.00    0.00    0.00       0
  0.000     2     6.000    0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00      0.00   0.00    0.00    0.00       0
  0.000     3    10.000    0.0000E+00     0.0000E+00     0.0000E+00     0.0000E+00      0.00   0.00    0.00    0.00       0
.
.
  0.500     1     2.000    0.1470E-14     0.4741E-15     0.0000E+00     0.6639E-16    100.00  32.25    0.00   67.75      72
  0.500     2     6.000    0.6979E-12     0.3339E-12     0.0000E+00     0.2427E-13    100.00  47.84    0.00   52.16      72
  0.500     3    10.000    0.2619E-09     0.1651E-09     0.0000E+00     0.6453E-11    100.00  63.04    0.00   36.96      72
.
.
  1.000     1     2.000    0.1304E-13     0.4897E-14     0.0000E+00     0.5429E-15    100.00  37.55    0.00   62.45     144
  1.000     2     6.000    0.2992E-11     0.1546E-11     0.0000E+00     0.9641E-13    100.00  51.67    0.00   48.33     144
  1.000     3    10.000    0.5484E-09     0.3554E-09     0.0000E+00     0.1287E-10    100.00  64.81    0.00   35.19     144
.
.
 30.000     1     2.000    0.1261E-15     0.3376E-16     0.0000E+00     0.6157E-17    100.00  26.77    0.00   73.23    4320
 30.000     2     6.000    0.1356E-13     0.5105E-14     0.0000E+00     0.5636E-15    100.00  37.65    0.00   62.35    4320
 30.000     3    10.000    0.1342E-11     0.6649E-12     0.0000E+00     0.4511E-13    100.00  49.56    0.00   50.44    4320
.
 30.000    80   318.000    0.5430E-03     0.4796E-03     0.0000E+00     0.4232E-05    100.00  88.31    0.00   11.69    4320
```

Fig. 22 Example of a WLSOCO.OUT file

```
* Output of concentrations and distribution percentages for the sediment subsystem
* under segment   80 of the water layer as a function of time and depth
* (middle of segment is at  318.000 m in water body)
*
* Percentage of total present calculated from
* mass per volume sediment
*
* Thickness top layer is  10.00 mm (upper  7 sediment segments)
*
*<====> <=>  <====>   <= concentrations ====================>  <= percentage ========> <====>
*  time  segm  depth        total    liq. phase  solid phase    total  liq.ph  sol.ph  timest
*                             cb*          clb           Xb
*     d            m       g.m-3        g.m-3        g.g-1        %       %       %
*
  0.000    1  0.0005  0.0000E+00   0.0000E+00   0.0000E+00     0.00    0.00    0.00       0
  0.000    2  0.0015  0.0000E+00   0.0000E+00   0.0000E+00     0.00    0.00    0.00       0
  0.000    3  0.0025  0.0000E+00   0.0000E+00   0.0000E+00     0.00    0.00    0.00       0
.
  0.000   14  0.0900  0.0000E+00   0.0000E+00   0.0000E+00     0.00    0.00    0.00       0
  0.000  top  0.0090  0.0000E+00   0.0000E+00   0.0000E+00     0.00    0.00    0.00       0

  0.500    1  0.0005  0.1042E+00   0.2789E-03   0.1299E-05   100.00    0.22   99.78      72
  0.500    2  0.0015  0.1791E-02   0.3056E-05   0.2235E-07   100.00    0.14   99.86      72
  0.500    3  0.0025  0.1212E-04   0.1187E-07   0.1513E-09   100.00    0.08   99.92      72
.
  0.500   14  0.0900  0.7798E-20   0.1000E-24   0.5198E-26   100.00    0.00  100.00      72
  0.500  top  0.0090  0.1060E-01   0.2820E-04   0.1322E-06   100.00    0.22   99.78      72

  1.000    1  0.0005  0.1868E+00   0.5335E-03   0.2329E-05   100.00    0.23   99.77     144
  1.000    2  0.0015  0.7051E-02   0.1401E-04   0.8799E-07   100.00    0.16   99.84     144
  1.000    3  0.0025  0.1148E-03   0.1445E-06   0.1434E-08   100.00    0.10   99.90     144
.
.
  1.000   14  0.0900  0.7798E-20   0.1000E-24   0.5198E-26   100.00    0.00  100.00     144
  1.000  top  0.0090  0.1940E-01   0.5477E-04   0.2419E-06   100.00    0.23   99.77     144
.
 30.000    1  0.0005  0.1896E+00   0.5425E-03   0.2364E-05   100.00    0.23   99.77    4320
 30.000    2  0.0015  0.1633E+00   0.4596E-03   0.2037E-05   100.00    0.23   99.77    4320
 30.000    3  0.0025  0.1088E+00   0.2927E-03   0.1357E-05   100.00    0.22   99.78    4320
.
 30.000   14  0.0900  0.7798E-20   0.1000E-24   0.5198E-26   100.00    0.00  100.00    4320
 30.000  top  0.0090  0.5475E-01   0.1498E-03   0.6829E-06   100.00    0.23   99.77    4320
```

Fig. 23 Example of a WBSCOxxx.OUT file

```
* Output of substance distribution in water layer and sediment
* as a function of time
*
*<====>  <= water layer ==============================>  <= sediment =====================>  <= whole system =>  <====>
*  time     total wl    dissolved     macroph.  susp.solid  total sed.    dissolved    solid sed        wl  sediment  timest
*     d            g            g            g           g           g            g            g         %         %
*
  0.000  0.3000E+00  0.2712E+00  0.0000E+00  0.2882E-01  0.0000E+00  0.0000E+00  0.0000E+00    100.00      0.00       0
  0.500  0.2662E+00  0.2404E+00  0.0000E+00  0.2585E-01  0.2159E-01  0.4707E-04  0.2154E-01     92.50      7.50      72
  1.000  0.2376E+00  0.2144E+00  0.0000E+00  0.2329E-01  0.3919E-01  0.9062E-04  0.3910E-01     85.84     14.16     144
  1.500  0.2135E+00  0.1924E+00  0.0000E+00  0.2111E-01  0.5345E-01  0.1270E-03  0.5332E-01     79.98     20.02     216
  2.000  0.1930E+00  0.1738E+00  0.0000E+00  0.1923E-01  0.6494E-01  0.1568E-03  0.6479E-01     74.82     25.18     288
  2.500  0.1755E+00  0.1579E+00  0.0000E+00  0.1762E-01  0.7419E-01  0.1807E-03  0.7401E-01     70.29     29.71     360
  3.000  0.1605E+00  0.1443E+00  0.0000E+00  0.1623E-01  0.8161E-01  0.1998E-03  0.8141E-01     66.29     33.71     432
.
.
 30.000  0.1578E-01  0.1386E-01  0.0000E+00  0.1922E-02  0.7940E-01  0.1725E-03  0.7923E-01     16.58     83.42    4320
```

Fig. 24 Example of a DBDIT.OUT file

```
* Output of substance distribution in water layer and sediment
* as a function of time at segment  80 of water layer (middle of segment is at  318.000 m)
*
*<====>  <= water layer ================================>  <= sediment ======================>  <= whole system =>  <====>
*  time      total wl    dissolved      macroph.   susp.solid  total sed.    dissolved  solid sed.   wat.lyr  sediment  timest
*     d       g.m'-1       g.m'-1        g.m'-1       g.m'-1      g.m'-1       g.m'-1      g.m'-1         %         %
*
   0.000  0.1000E-02  0.9039E-03  0.0000E+00  0.9608E-04  0.0000E+00  0.0000E+00  0.0000E+00    100.00      0.00       0
   0.500  0.9024E-03  0.8149E-03  0.0000E+00  0.8752E-04  0.7257E-04  0.1583E-06  0.7241E-04     92.56      7.44      72
   1.000  0.8194E-03  0.7392E-03  0.0000E+00  0.8017E-04  0.1328E-03  0.3075E-06  0.1325E-03     86.05     13.95     144
   1.500  0.7488E-03  0.6749E-03  0.0000E+00  0.7387E-04  0.1826E-03  0.4350E-06  0.1822E-03     80.39     19.61     216
   2.000  0.6885E-03  0.6201E-03  0.0000E+00  0.6844E-04  0.2237E-03  0.5414E-06  0.2232E-03     75.47     24.53     288
   2.500  0.6369E-03  0.5731E-03  0.0000E+00  0.6376E-04  0.2577E-03  0.6295E-06  0.2571E-03     71.19     28.81     360
   3.000  0.5923E-03  0.5326E-03  0.0000E+00  0.5969E-04  0.2857E-03  0.7020E-06  0.2850E-03     67.46     32.54     432
.
.
  30.000  0.1140E-03  0.1007E-03  0.0000E+00  0.1333E-04  0.3774E-03  0.8465E-06  0.3765E-03     23.21     76.79    4320
```

Fig. 25 Example of a DBxxx.OUT file

5.5 Exposure concentrations: ECxxx.OUT

This file shows the exposure concentrations of the pesticide in the water layer and the top layer of the sediment under water layer segment xxx (see Fig. 26). For each time step of output, it considers the momentary concentrations (column 2), the Time Weighed Average Exposure Concentrations TWAECs (columns 3-6) and the depth-weighed average concentration in the top layer of the sediment (column 7).

The table at the bottom of the file shows for each of the exposure periods (column 1), the time of occurrence (column 2) of, and the maximum exposure concentrations (column 3) in the segment xxx.

```
 * Exposure concentrations in water layer and momentary total concentrations
 * in top layer sediment (depth-weighed average of top  10.0 mm)
 * at segment  80 of water layer (middle of segment at  318.000 m)
 * (for calculation of TWAECs it is assumed that concentration in water layer is
zero in 28 days
 * before start of simulation
 *
 *<=====>  <= water layer ==========================>  <sediment>   <=======>
 *  time    momentary      TWAEC4      TWAEC21      TWAEC28   momentary  time step
 *     d        g.m-3        g.m-3        g.m-3        g.m-3        g.m-3
 *
   0.000    0.430E-02           -            -            -   0.000E+00          0
   0.500    0.388E-02   0.514E-03   0.979E-04   0.735E-04   0.106E-01         72
   1.000    0.352E-02   0.976E-03   0.186E-03   0.139E-03   0.194E-01        144
   1.500    0.321E-02   0.140E-02   0.266E-03   0.199E-03   0.267E-01        216
   2.000    0.295E-02   0.178E-02   0.339E-03   0.254E-03   0.327E-01        288
   2.500    0.273E-02   0.214E-02   0.407E-03   0.305E-03   0.376E-01        360
   3.000    0.254E-02   0.246E-02   0.469E-03   0.352E-03   0.417E-01        432
 *
 *
  30.000    0.480E-03   0.527E-03   0.821E-03   0.111E-02   0.548E-01       4320


 * Maximal exposure concentrations in water layer for 0, 4, 21 and 28 days
 * at   318.000 m in water body
 *
 *  exp. time     time of occur.     exp.conc.
 *           d                d        g.m-3
 *
             0             0.00   0.4304E-02
             4             4.00   0.3057E-02
            21            21.00   0.1564E-02
            28            28.00   0.1327E-02
```

Fig. 26 Example of a ECxxx.OUT file

6 The graphical user interface (TOXSWA-GUI)

6.1 Introduction

This chapter describes the graphical user interface (GUI) for the TOXSWA simulation program. The GUI is a tool to create input files, to start the simulation and view the results in the output files via standard graphs.

The TOXSWA-GUI is independent of the TOXSWA simulation program; it is a stand-alone program. You do not need to have the TOXSWA program at all. The simulation, can be run from the GUI; the GUI calls the TOXSWA program. It seems as if the GUI and the simulation have been integrated. Section 6.2 describes how the GUI can be used.

Section 6.3 describes the main page (TOXSWA page), that appears on your screen after starting the GUI. This is the control centre of the GUI, all operations start from this page. The philosophy behind the TOXSWA-GUI is that the user wants to simulate a certain pesticide for a certain scenario, e.g. a pesticide to be authorized for the Dutch standard spring scenario. Section 6.4 describes how to enter the scenario parameters, and Section 6.5 describes how to enter the pesticide parameters. Running TOXSWA is described in Section 6.6. Section 6.7 describes how the output of TOXSWA can be viewed graphically, including how you can compare two simulations and how to compare simulations with measurements. Finally, Section 6.8 describes how you can run TOXSWA for a series of runs.

6.2 Using the GUI

This section describes some basic principles of the GUI.

Navigating
The data needed to run the simulation have been distributed between a number of pages, or >tabs*. Each of these pages has its own >tab*, placed at the top of the main window. Each tab has its own name, for example, APesticide≅ or AHydrology≅. These names indicate the kind of data that can be edited. Clicking on a tab makes the GUI switch to a different page.

Error handling
If you typed in an illegal value (incorrectly typed or outside the range), the GUI responds almost immediately[1]. You must enter a legal value before you can continue to edit other values. Wrongly spelled values (e.g. a letter instead of a digit) or values beyond a TOXSWA-specific range result in error messages. There

[1] The GUI responds when you 'leave' the editbox. You leave the editbox, for instance, by clicking another editbox of button. This means, you have to enter a legal value before you can continue.

may be errors that can only be found by the TOXSWA simulation program. The GUI has no way of knowing this type of errors, so you should always check the results of a TOXSWA run.

Help
Help on selecting or estimating proper values for parameters is provided via clicking on "Help" from the menu bar. After clicking on "Contents" a list is shown of parameters for which help is available. You can select a topic. When you enter data help can be asked on a specific parameter by selecting its edit box, followed by typing < F1 > (not all parameters). The help provided is the same as the help on parameter estimation in Chapter 8 of this manual.

6.3 TOXSWA page, control centre of the GUI

The GUI opens on the TOXSWA page. From this page you can: (i) go to the pages where data for the input files have to be entered, (ii) start a simulation, (iii) view output of a simulation run, and (iv) set a batch for running TOXSWA simulations. The three operations mentioned first, handle the scenario and the pesticide that are shown in the white boxes inside the *run* section (see Fig. 27). [2]

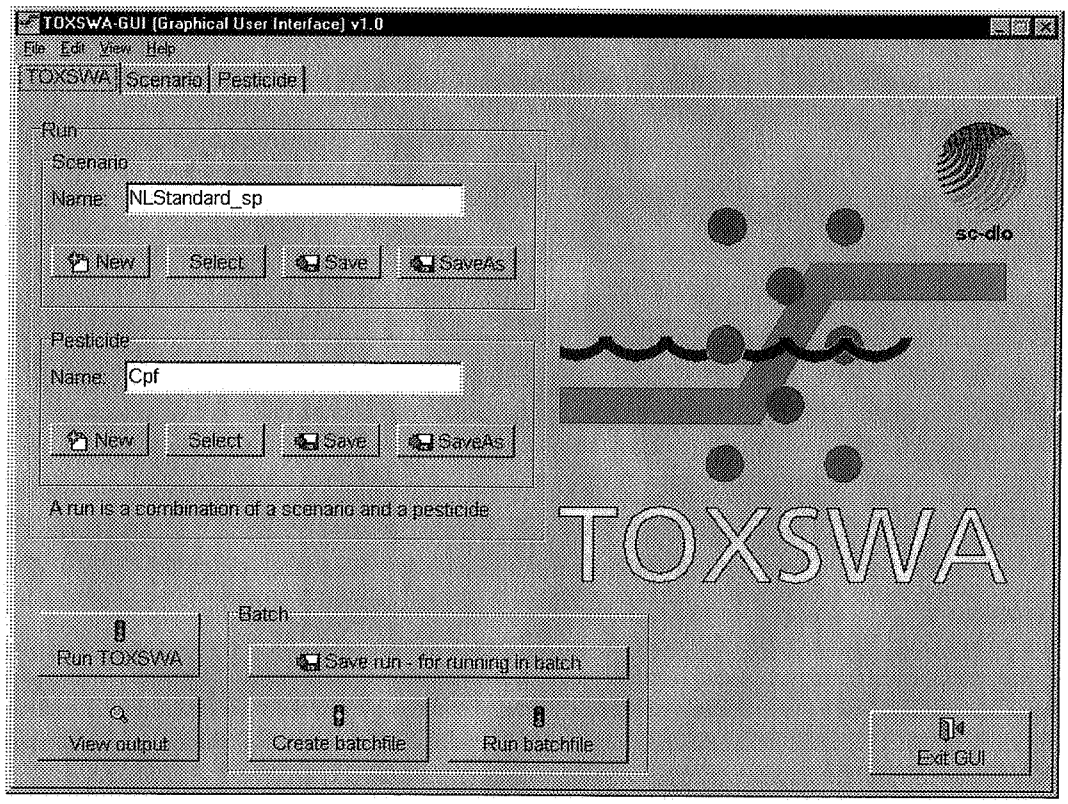

Fig. 27 The TOXSWA page of the TOXSWA-GUI

[2] The names of the scenario and the pesticide equal the names of directories in which the input files are stored. After clicking "Run TOXSWA", a directory named 'name of scenario'+'name of pesticide' is made by the GUI. The output of the simulation run is stored in this directory.

The three tabs at the top of the page enable you to move between the three pages:

TOXSWA – This page is the control centre of the GUI, from this page all main operations can be directed.

Scenario – This page is the entry page for editing and viewing scenario input parameters.

Pesticide – This page is the entry page for editing and viewing pesticide input parameters.

The Scenario page and the Pesticide page are described in Section 6.4 and Section 6.5, respectively. The buttons of the TOXSWA page have been described in this section.

Run section
The scenario and pesticide currently stored in the GUI are shown in the white boxes. The buttons in the *run* section, and how to handle them, have been described below:

"New" sets all input parameters to default values (Dutch standard spring scenario / example pesticide chlorpyrifos).

"Select" to select a scenario or pesticide that was saved before: click the "Select" button, then select by double-clicking the name of the scenario or pesticide from the list that is shown in the left box (this is also the name of a map on your computer).

"Save" to save input parameters edited under the name of the scenario or pesticide that is shown in the white box.

"SaveAs" to save input parameters edited under a new name (scenario or pesticide): click the "Save as" button, type the name of the scenario or pesticide in the upper white box preceded by a back slash (the name becomes also a directory).

Run TOXSWA
Click "Run TOXSWA" to start the simulation. See Section 6.6 for a further description.

View output
Click "View output" to view graphical output of a simulation (the combination of the scenario and pesticide shown in the white boxes). A detailed description is given in Section 6.7

Batch section
Buttons to prepare and run batch files, for execution of a series of simulation runs. A detailed description is given in Section 6.8

Exit
Click to exit the GUI.

6.4 Entering scenario input

The scenario parameters concern all parameters that define the system physically (the water body) and numerically as needed for a simulation (e.g. time step). The scenario page contains the following (sub)pages (see Fig. 28):

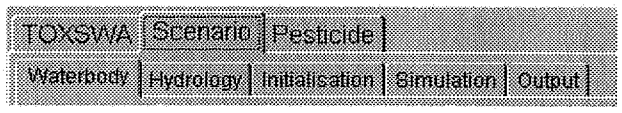

Fig. 28 The subpages of the Scenario page of the TOXSWA-GUI

Water body - This page allows you to edit all water body (water layer and sediment) characteristics, including geometry and lengths of the segments (see Section 6.4.1).

Hydrology - This page contains all hydrological information, such as water flow velocity and seepage, and the temperature (see Section 6.4.2).

Initialisation - On this page you can easily change the initial concentrations in particular segments of the water layer and the sediment (see Section 6.4.3).

Simulation - On this page you can edit time aspects of the simulation, for instance, the duration of the simulation or the points in time at which output is desired. You can also select the segments for which output is wanted (see Section 6.4.4).

Output – This page allows you to select the output files that you want to be generated by TOXSWA (see Section 6.4.5).

6.4.1 Water body page

On the Water body page (see Fig. 29) you can:
- change the dimensions and side slope of the water body,
- edit the segments within the water layer,
- edit the segments within the sediment, and
- change some water body characteristics (such as the dry weight of the macrophytes per m^2 bottom area).

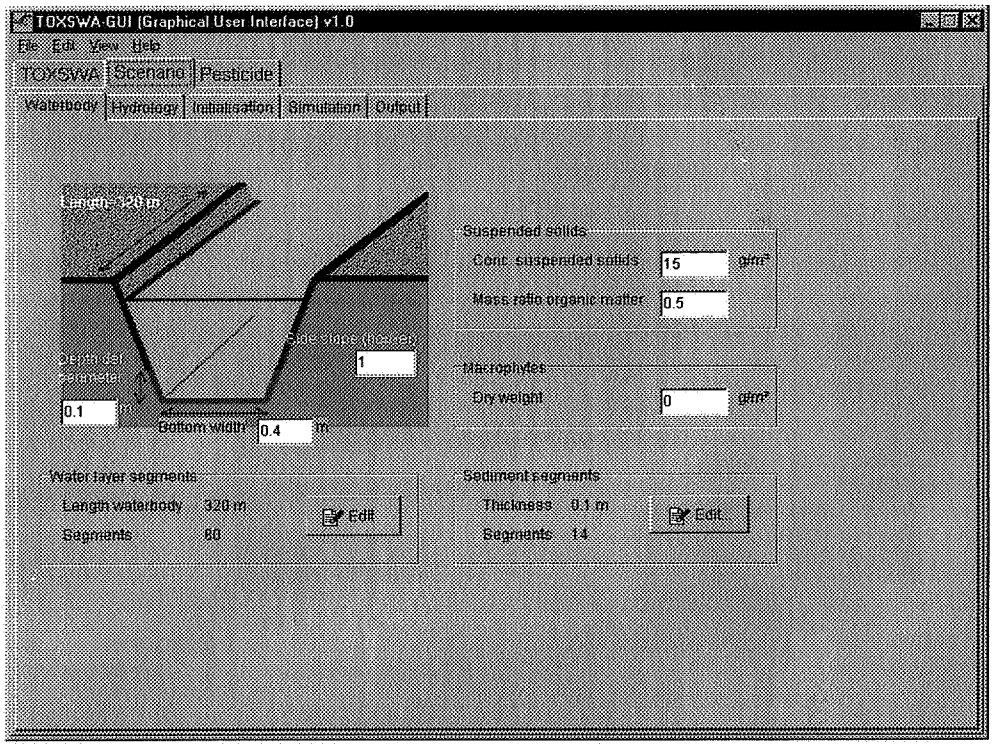

Fig. 29 Example of the Water body page of the TOXSWA GUI

To change the bottom width, the depth of the water layer, the side slope or the length of the draining plot, you have to enter the values in the edit boxes.

To edit the segments within the water body or the length of the water body, press the AEdit≅ button in the AWater layer segments≅ section. There is also an AEdit≅ button in the Sediment section.

Editing segments in the sediment is similar to those in the water layer, except that there are more segment attributes that can be entered (porosity, tortuosity, etc.). To change the number of top layer segments for which the accumulated pesticide mass is to be calculated, change the value in edit box.

To remove a segment from the list, you must first select the segment and then press the ARemove≅ button. The segment will disappear from the list. The AClear list≅ button can be used to remove all segments but one.

To generate a set of segments, you can click the AGenerate≅ button. You are then presented a choice of distributions: a fixed number of segments uniformly distributed, a quadratic distribution (only for sediment) or segments of a fixed length. If you click on OK, the GUI will generate a set of segments.

The length can be changed by entering the value in the edit box (in the segments dialogue window). If there are segments beyond the length, the GUI asks you

whether or not these segments should be deleted. If you choose not to do so, the length will remain unchanged.
Another way to change the length is by scaling the entire region. This means that length and segments will be equally scaled. If you press the AScale≅ button, you can enter the scaling factor by which the length and segment lengths are to be multiplied. This allows you to reduce the size easily without losing segments.

6.4.2 Hydrology page

The page shows some edit boxes in which you can enter hydrological values, such as flow velocity, the dispersion coefficient, the seepage, and the concentration in the incoming seepage water (see Fig. 30). Also the temperature in the water body system can be entered.

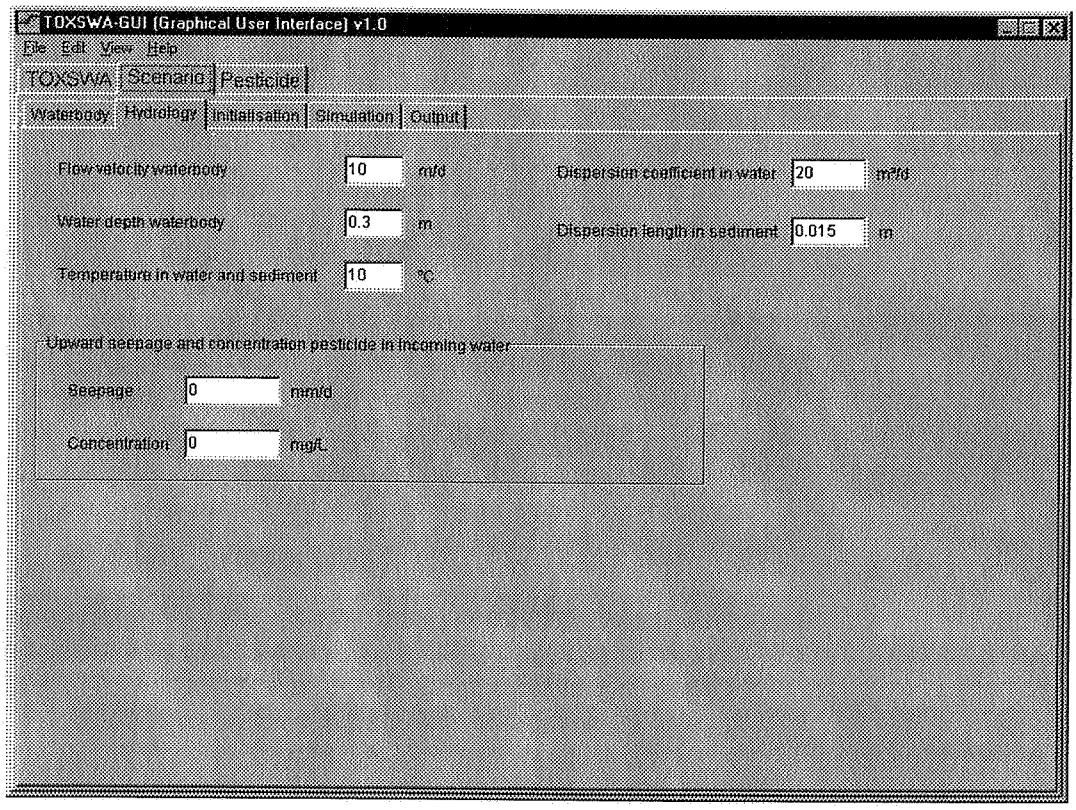

Fig. 30 Example of the Hydology page of the TOXSWA-GUI

6.4.3 Initialisation page

On this page you can quickly set and change the initial concentrations in the segments of the water layer and the sediment (see Fig. 31).

By clicking the radio buttons, you can select which segments you want to change; water layer or sediment segments. The list box shows all segments and their initial concentrations.

To change the initial concentration in a specific segment enter the concentration in the concentration edit box.

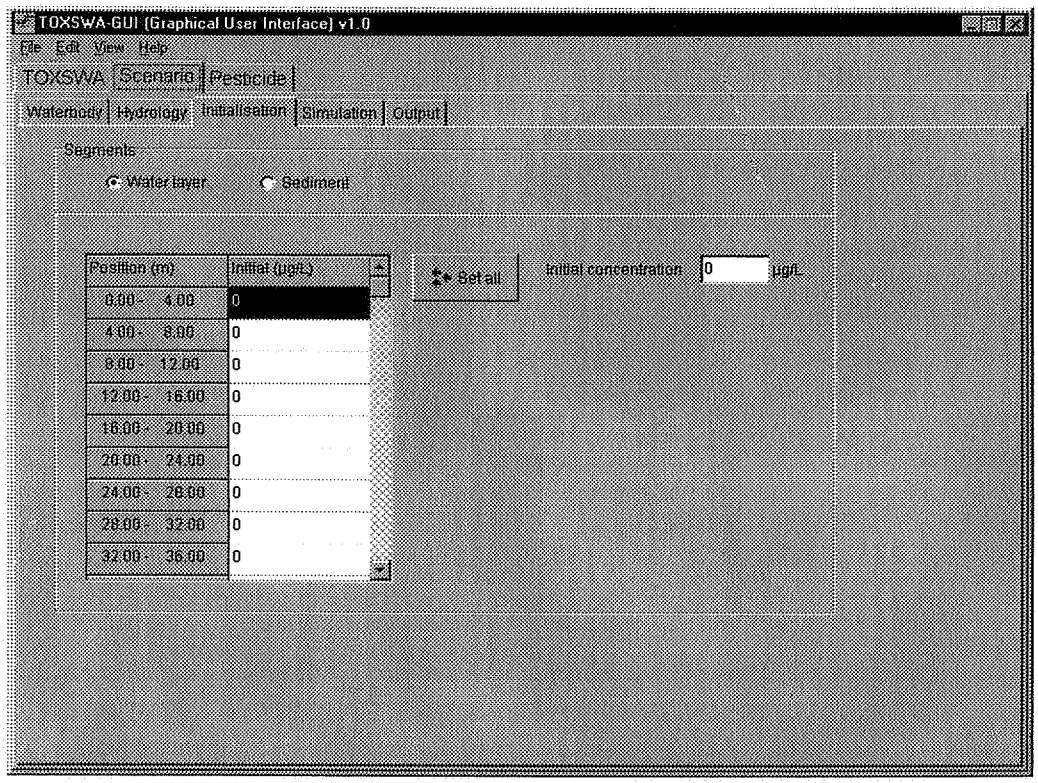

Fig. 31 Example of the Initialisation page of the TOXSWA-GUI

To set all initial concentrations to the same value, enter the value in the edit box and press the ASet all≅ button.

6.4.4 Simulation page

The Simulation page is divided into three sections: Time, Output Time, Output Segments (see Fig. 32).

In the Time section you can enter the total time for which the simulation should run. The calculation time step for the simulation can be changed by entering the value (in seconds) in the edit box below the total time.

In the Output Time section you can enter a fixed time interval at which output is to be generated.

You can select the segments for which output is wanted in the Output Segments section. This section shows two list boxes: one for segments selected for output and one for the remaining segments. Segments can be moved from one list to the other by selecting them and clicking the appropriate button. Note that average exposure concentrations will be calculated for the segments selected here.

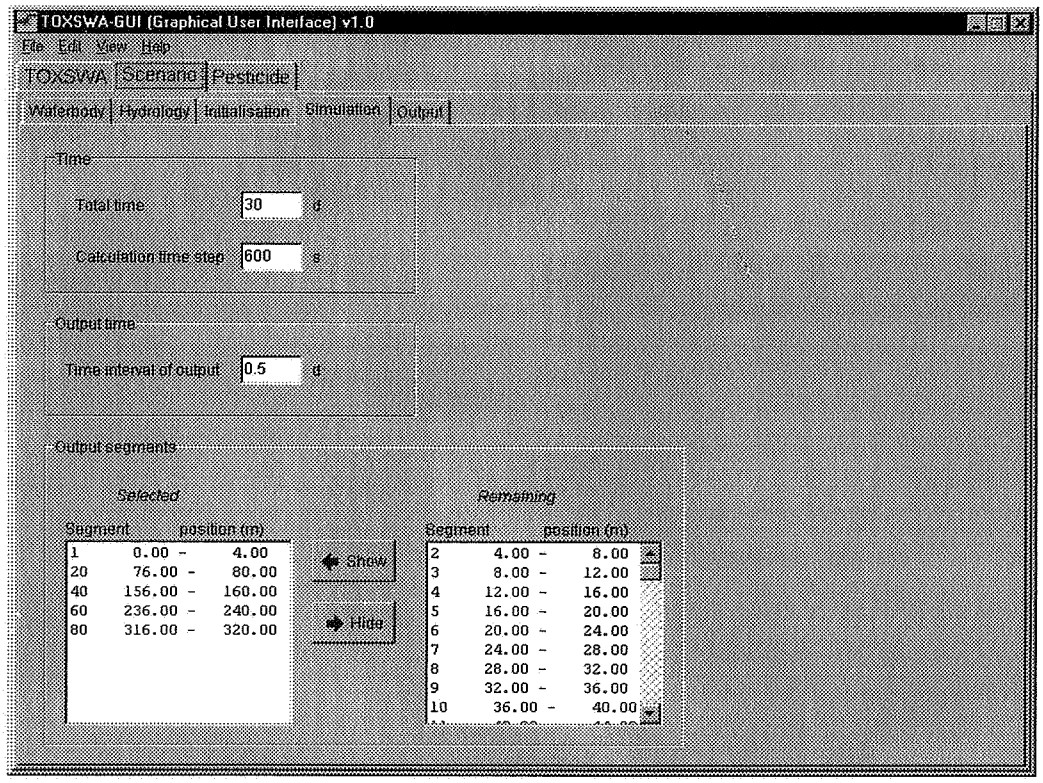

Fig. 32 Example of the Simulation page of theTOXSWA-GUI

For example, if you want to select a segment for output, first select the segment in the remaining-segments list. Then click the AShow≅ button. The segment will be 'moved' from one list to the other.

You can obtain the following output files for the segments selected (segment xxx); `wbscoxxx.out` (concentrations in the sediment subsystem xxx), `wlmbxxx.out` (mass balance for segment water layer xxx), `wbmbxxx.out` (mass balance for sediment subsystem xxx), `dbxxx.out` (distribution between compartments in sediment subsystem xxx), and `ecxxx.out` (exposure concentrations in water layer segment and of toplayer sediment) subsytem. To produce these files during simulation the corresponding output has to be selected in the Output page (see Section 6.4.5).

6.4.5 Output page

You can select which output files have to be created during the simulation run. If you want to be able to view all graphs defined in the GUI, you need to select the option Needed for viewing output with GUI (see Fig. 33).

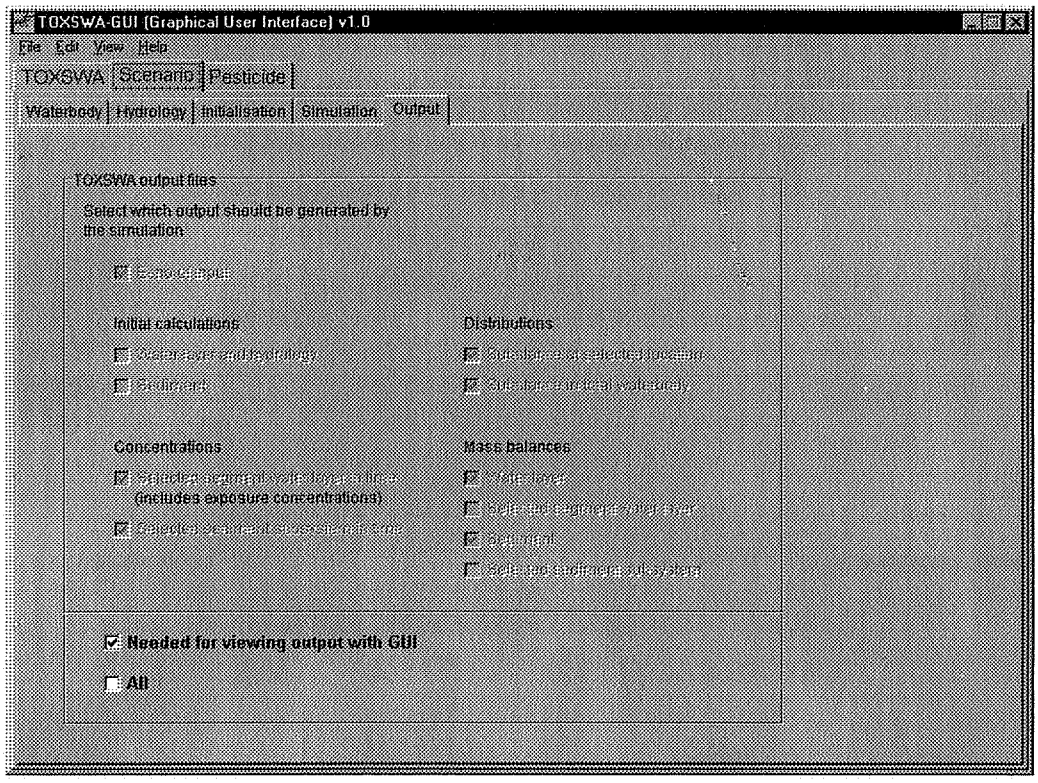

Fig. 33 Example of the Output page of the TOXSWA-GUI

6.5 Entering pesticide input

All parameters concerning the pesticide can be edited on the Pesticide page, which has four subpages (see Fig. 34). Each subpage can be selected by clicking on its tab at the top of the Pesticide page.

Transformation – This page allows you to edit parameters for transformation in water and sediment (see Section 6.5.1).

Sorption – This page allows you to edit sorption parameters for macrophytes, suspended solids and sediment organic matter (see Section 6.5.2).

Volatilization – This page allows you to edit volatilization parameters for the water layer, and for diffusion in the sediment (see Section 6.5.3).

Loading – This page allows you to edit input for the pesticide loadings; the time of loading, the mass and the stretch of the water body onto which the pesticide is deposited (see Section 6.5.4).

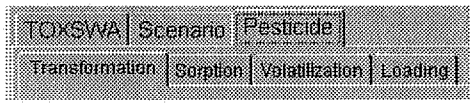

Fig. 34 The Pesticide page of the TOXSWA-GUI

6.5.1 Transformation page

The page shows some edit boxes in which you can enter the half-lives for water and sediment, and the activation energy for transformation (see Fig. 35).

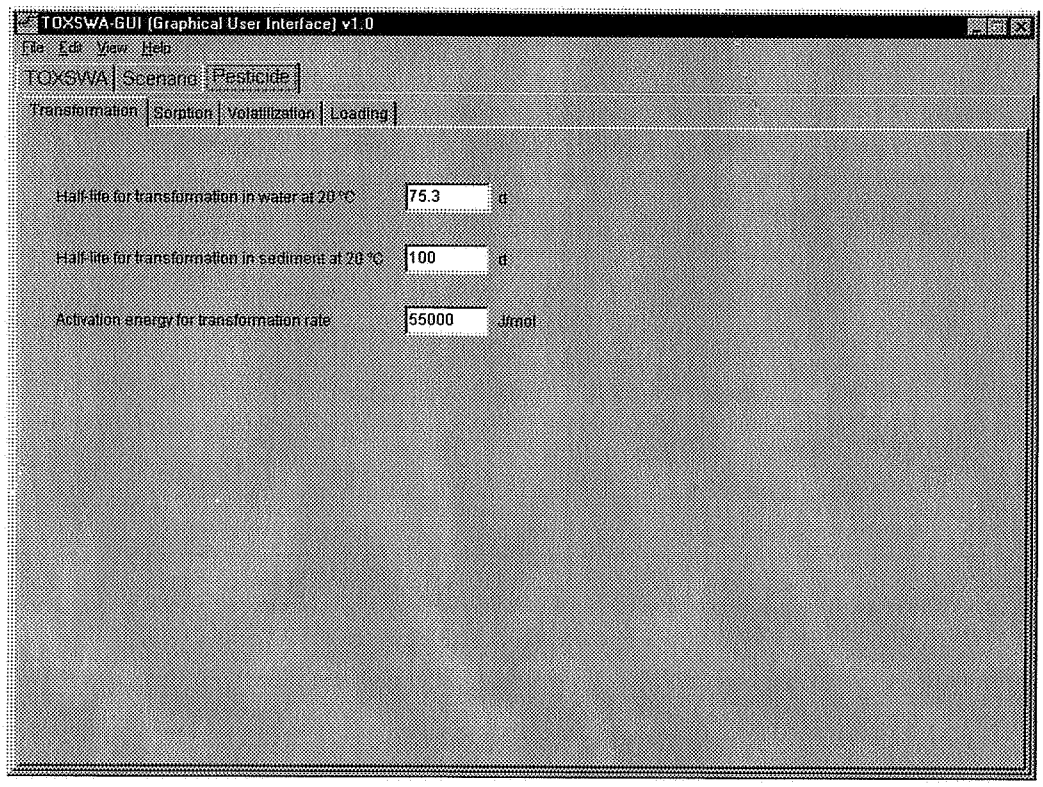

Fig. 35 Example of the Transformation page of theTOXSWA-GUI

6.5.2 Sorption page

This page shows three sections: suspended solids, sediment and macrophytes (see Fig. 36). In each of the three sections, there are edit boxes in which you can enter the sorption coefficients. For the suspended solids and the sediment organic matter Freundlich sorption parameters can be entered as well.

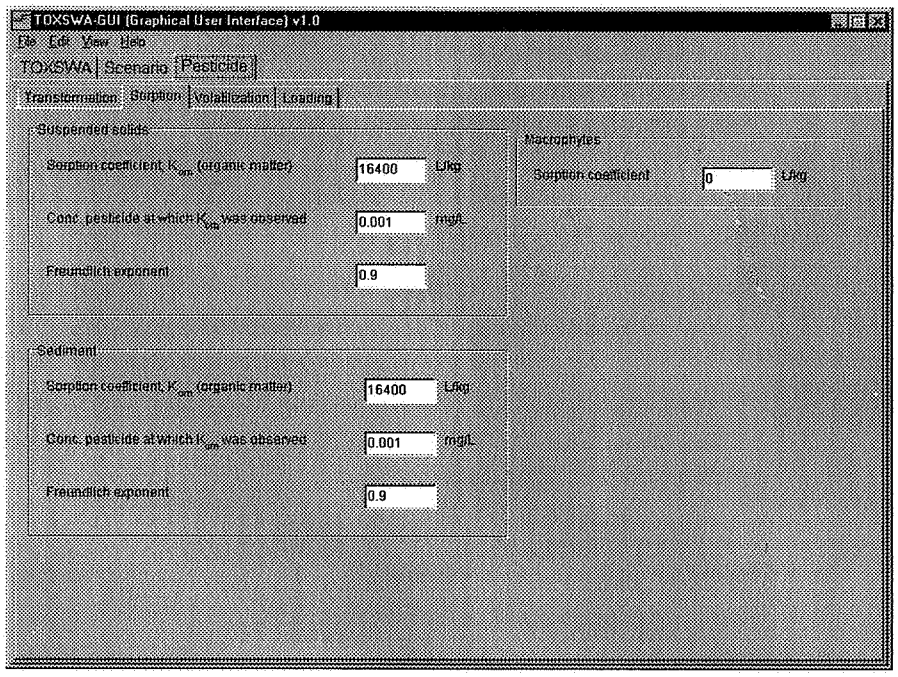

Fig. 36 Example of the Sorption page of theTOXSWA-GUI

6.5.3 Volatilization page

The Volatilization page is divided into three sections: Saturated gas pressure, Solubility and Exchange coefficients (see fig. 37). The Molecular mass and Diffusion coefficient can be entered in two edit boxes outside the three sections.

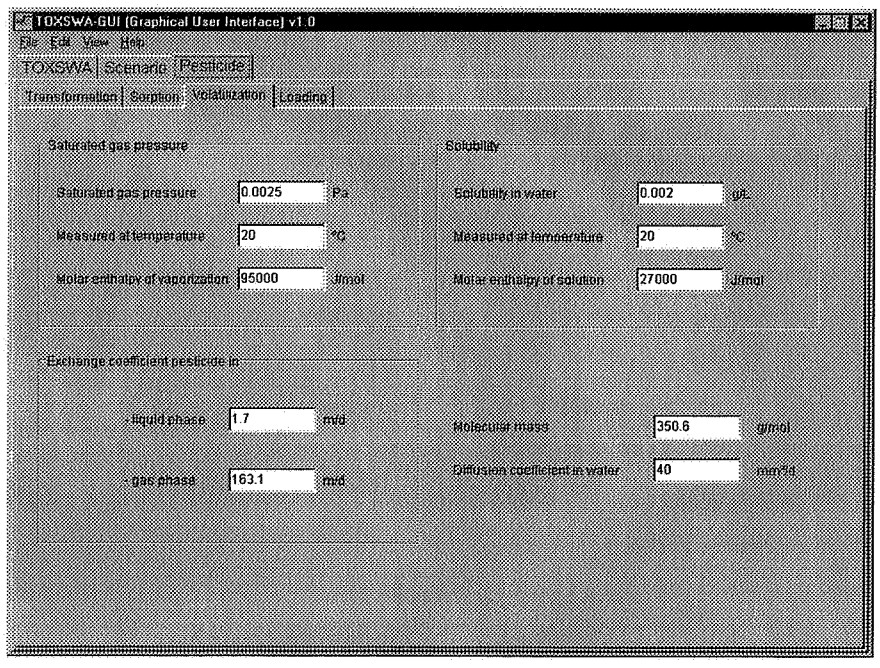

Fig. 37 Example of the Volatilization page of theTOXSWA-GUI

In the Saturated gas pressure and Solubility sections you can enter the saturated vapour pressure and the solubility respective, and their molar enthalpies and temperatures at which the enthalpies were measured.

In the Exchange coefficients section, you can enter the exchange coefficients for the gas and liquid phase.

6.5.4 Loading page

On the Loadings page, the entry time, the start position and the end position in the water body, and the mass of the loading (per m^2 water surface area) have to be entered in the table (see Fig. 38).

To add a loading, press the "Insert" button. The GUI inserts a copy of the first loading, directly below the first loading. Then you can edit the values in this new line. Take care that the loadings must be given in chronological order.

To remove a loading from the list, you must first select the loading and then press the ARemove≅ button. The loading will disappear from the list.

The AClear list≅ button can be used to remove all loadings, except one default loading.

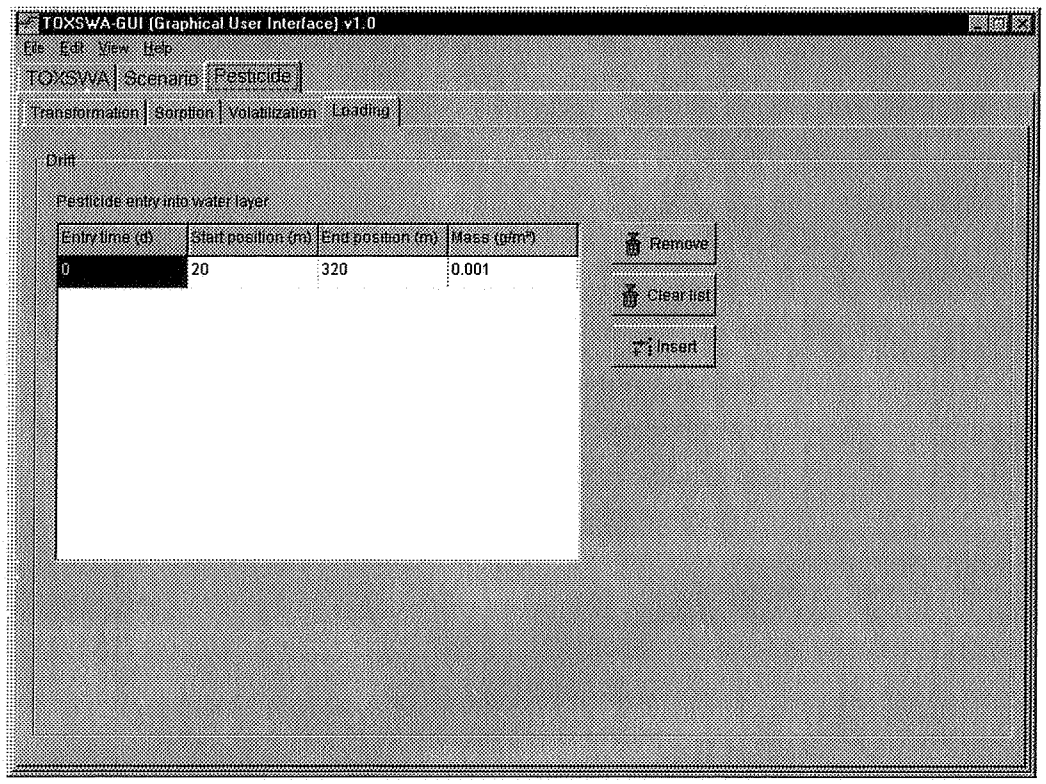

Fig. 38 Example of the Loadings page of theTOXSWA-GUI

6.6 Running the simulation

To run a TOXSWA simulation select the scenario and the pesticide you want to combine (see Section 6.2). Press the "Run TOXSWA" button. A DOS session (black screen) is started up and messages produced by TOXSWA during simulation are shown. When the run has terminated, the DOS session ends. Depending on the operating system of your computer you have to confirm that the simulation was finished (Windows95), or the DOS screen disappears automatically (WindowsNT).

When the simulation is finished a message is shown in the DOS box. When errors or warnings occurred, the `message.out` file should be read. Use the explorer to go to the directory

`c:\toxswa\runs\`*`name_scenario+name_pesticide`*

to view the contents of `message.out`.

Note that a run may take several minutes (see Chapter 9). Section 7.2 discusses message handling during simulation. After the run has terminated you can view the results (see Section 6.7).

Don't use the "+" symbol in the name of the scenario or the name of the pesticide. The GUI may not be able to find the results of the run because the run name will contain two "+" symbols.

6.7 Viewing output

By pressing the 'View Output' button you can inspect the simulation results in charts (see Fig. 39).

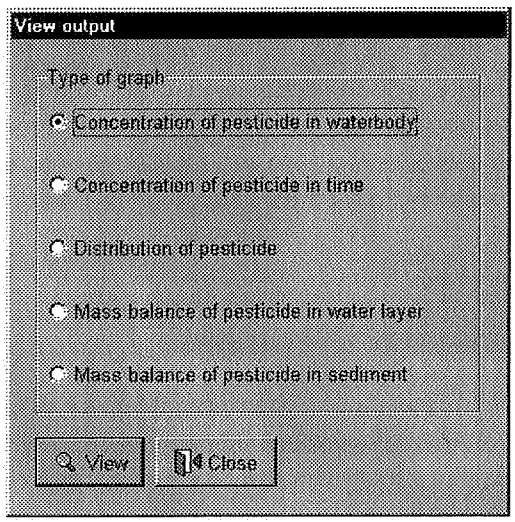

Fig. 39 Example of the View output screen of the TOXSWA-GUI

You can view, manipulate, compare and print charts. You can select five different chart types:

Concentration of pesticide in water body - The concentration in the water layer is given as a function of the distance in the water layer. The concentration in the sediment is given a function of depth in three sediment subsystems.

Concentration of pesticide in time - The concentration in the water layer is given as a function of time for maximally 9 water layer segments. The concentration in the top layer of the sediment is given as a function of time in three sediment subsystems. Also shown is a table with the acute and chronic exposure concentrations.

Distribution of pesticide – For the entire water layer the distribution of the pesticide between the compartments is given as a function of time. For the sediment the distribution of the pesticide is given as function of time in three sediment subsystems.

Mass balance of pesticide in water layer – The pesticide mass balance of the entire water layer of the water body is given as a function of time.

Mass balance of pesticide in sediment – the pesticide mass balance of the whole sediment layer of the water body is shown as a function of time.

To select the chart you want to see, mark its checkbox. The GUI shows selected chart after pressing the "View" button.

Note that for the graphs that present results for sediment subsystems, only results can be shown for subsystems that have been selected for output at the start of the simulation (see Section 6.4.4 Output segments). This also applies for the table presented next to the *Concentration of pesticide in time* graph; only exposure concentrations for segments beforehand selected can be shown.

Section 6.7.1 shows how to manipulate the graphs with the tools provided by the GUI. In the graphs *Concentration of pesticide in water body* and *Concentration of pesticide in time* the simulated curves can be compared with other simulation results, or with measurements. These options have been described in Section 6.7.2.

6.7.1 Using the GUI for viewing graphs

Figure 40 shows an example of a graph page. Each of the charts can be enlarged and be presented in a single window by clicking the "Zoom" button (the button with a lens icon).

Charts can be printed by pressing the "Print" button (with the printer icon). Charts can be saved digitally as a bitmap file for import in other applications, by pressing

the "Save as BMP" button. Values that were used to draw the chart can be examined by pressing the "Table" button.

To zoom in on a specific part of the chart, you must click with the cursor at the left side at the top-left corner of that part and drag the cursor to the bottom-right corner. To undo the zooming, drag the cursor from bottom-right to top-left.

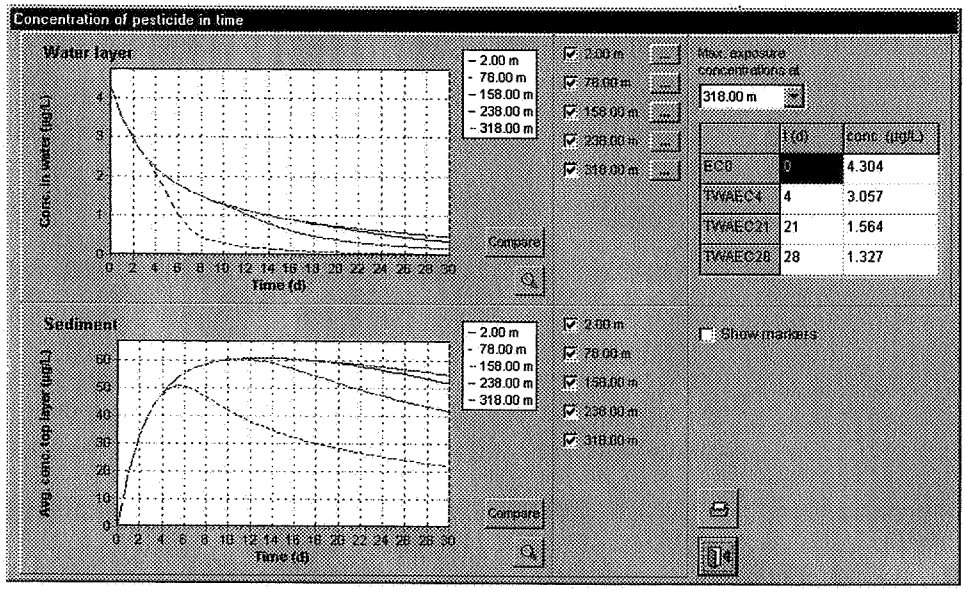

Fig. 40 Example of a graph page of theTOXSWA-GUI

The axes of the graphs can be customized. The title along the axis, the axis range and the tic steps along the axis can be altered. This can be done only after you have zoomed in to a graph in a single window (press the "Zoom" button). To manipulate the axis of a graph press the "Axis" button. Then two sections are shown, one for the X-axis, and another for the Y-axis. For both axis you can enter the start and end value of the axis, the title of the axis, the major tick step and the number of minor ticks. Note that the major tick step is a numerical values of a certain dimension (e.g. 25 m), and that the number of minor ticks indicates the number of tics between two major tics (hence without dimension).

The tools described below are not available for all graphs, in most cases they are only available for the graphs *Concentration of pesticide in water body* and *Concentration of pesticide in time.*

Segments or times other than the displayed ones can be selected by pressing the buttons with three dots. A list of all possible segments or times is shown then. You can select one of them. Each curve displayed in a graph can be switched off and on via a checkbox in the legend of the graph.

Showing the markers of the curves can be switched on and off with the "Show markers" checkbox.

A simulation can be compared with other simulation results, or with measurements by clicking the "Compare" button. This option is available only for the graphs *Concentration of pesticide in water body* and *Concentration of pesticide in time*.

6.7.2 Comparing two simulations or a simulation with experimental data

This section describes how the compare option of the GUI can be used. Two simulations can be compared, or a simulation can be compared with measurements. This option is available only for the graphs *Concentration of pesticide in water body* and *Concentration of pesticide in time*.

To compare simulations or compare a simulation with measurements click the "Compare" button (in some graphs shortened to "Comp.").

First, at the top of the page, you have to select if you want to compare simulations ("Two runs") or compare a simulation run with measured data ("Run with measured data"). Figure 41 shows an example of the Compare page.

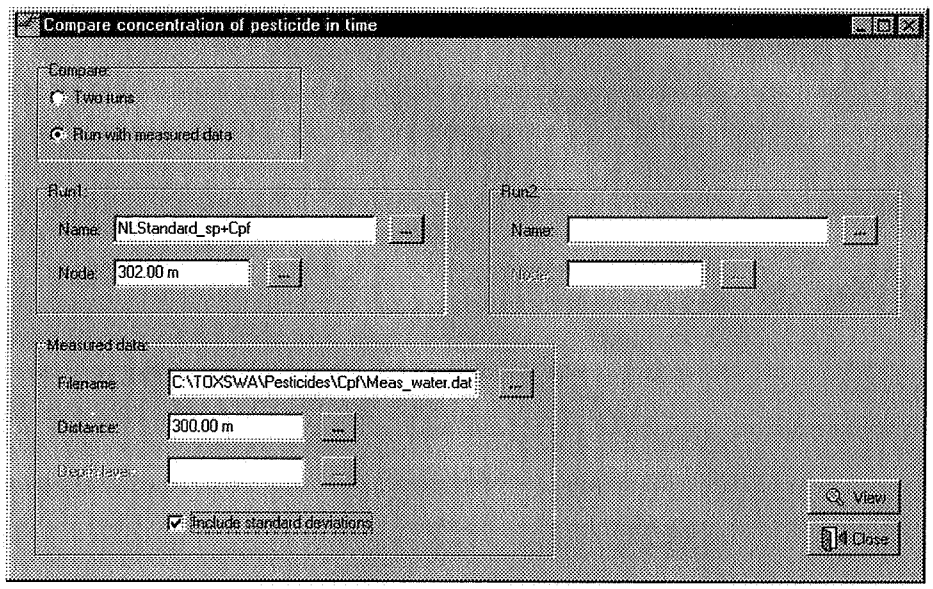

Fig. 41 Example of the Compare page of theTOXSWA-GUI

The "Run 1" section shows the simulation run that is considered, the name of the scenario plus the name of the pesticide are shown in the "name" box. Other simulation results can be selected by pressing the button with three dots. Further input depends on the type of graph that is compared:
Concentration in the water body: In the "Time" box a time step should be selected, and no "Node" has to be selected. When concentrations in the sediment are compared, a "Time" and a "Node" (= segment) have to be selected.

Concentration in time: Only the "Node" has to be selected, indicating for which water layer segment (water layer) or sediment subsystem (sediment) the concentrations are compared.
When two simulation runs are compared, data should be entered in the "Run 2" section. Select a simulation run from the list. For entering the "Time" and "Node" see the paragraph above.

When a simulation run is compared with measurements, data should be entered in the "Measured data" section. First, select the file with measured data by pressing the button with three dots behind the "Filename" box (a description of the data file is given below). Further input depends on the type of graph that is compared:
Concentration in water body: When concentrations in the water layer are compared, the "Sample period" should be selected, and for comparing concentrations in the sediment a "Time" should be selected.
Concentration in time: When concentrations in the water layer are compared, the "Distance" should be selected, and for comparing concentrations in the sediment a "Depth layer" should be selected.

The checkbox "Include standard deviations" can be marked when standard deviations are given in the data file.

The formats of the data files are demonstrated for the water layer in Figure 42 and for the sediment in Figure 43. You can make your own data files by using the shown formats. Always 5 columns should be given in the file. When the standard deviations are not known, dummy values should be entered. In the water layer data file the sample period should be given, because in flowing systems, water is often sampled proportionally to the flow rate. When samples are taken immediately, the start and end time of the sampling period are equal.

```
* File with measured data:
* concentration in water layer
*
* The last column is only needed for the option
* '+ Standard deviations'
*
* Sample time  Distance  Average     S.d.
* (d)            (m)       (mg/L)     (mg/L)
* start    end
    0.0     0.0    300.     0.0045     0.0008
    5.0     5.0    300.     0.0029     0.0011
   10.0    10.0    300.     0.0021     0.0008
   15.0    15.0    300.     0.0018     0.0006
   20.0    20.0    300.     0.0018     0.0005
   25.0    25.0    300.     0.0009     0.0003
   30.0    30.0    300.     0.0005     0.0005
```

Fig. 42 Example of the data file with measurements on the concentration in the water layer

```
* File with measured data:

* Total concentration in sediment
*
* The last column is only needed for the option
* '+ Standard deviations'
*
* Time      Depth layer      Average    S.D.
* (d)       (m)              (mg/L)     (mg/L)
*           from     to
    0.0     0.0      0.01     0.0        0.0
    5.0     0.0      0.01     0.043      0.010
   10.0     0.0      0.01     0.050      0.012
   15.0     0.0      0.01     0.046      0.008
   20.0     0.0      0.01     0.042      0.013
   25.0     0.0      0.01     0.038      0.013
   30.0     0.0      0.01     0.026      0.009
```

Fig. 43 Example of the data file with measurements on the concentration in the sediment

Press "View" to display the graph on your screen. The axes of the graph can be customized and the graph can be printed and saved as a bitmap by using the buttons a the bottom of the page.

6.8 Batch execution with TOXSWA

The GUI can create and run batch files for execution of a series of predefined simulation runs. The "Batch" section at the TOXSWA page contains the buttons needed: "Save run for running in batch", "Create batch file" and "Run batch file" (see Fig. 27).

Before creating a batch file, you need to save the individual runs that you want to be executed. A run is a combination of a scenario and a pesticide. To save a run: select a scenario and a pesticide in the 'Run" section, then press the "Save run for running in batch" button. The background of this operation is that a run name and a directory `c:\toxswa\runs\name_scenario+name_pesticide` is created.

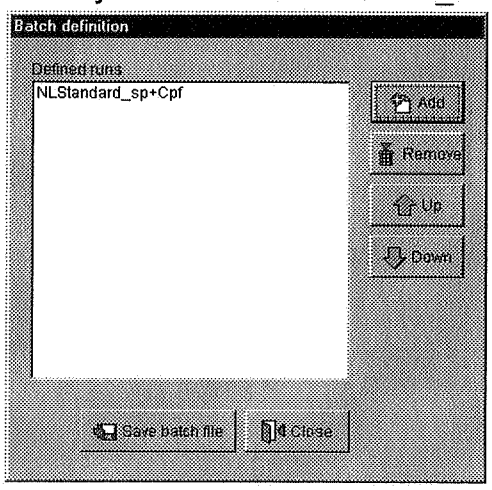

Fig. 44 Example of the Compare page of the TOXSWA-GUI

To create a batch file you must click the "Create batch files" button. The GUI shows an empty box to which runs can be added. When a couple of runs have been added, a run can be removed, moved up and moved down in the list of runs (see Fig. 44). The batch file can be saved and you can exit the dialog.

Runs can be added by pressing the "Add" button. The runs (also maps on your computer) to be included in the batch file are shown in the second list box that appears on your screen. Select a run by double clicking on the name of the run.

To remove a run from the list, you must select a run and press the "Remove" button.

The order of the runs in the list, is the order in which they will be executed. To change the position of a run, you must select a run and use the "Up" and "Down" buttons.

By pressing "Save batch file" the GUI creates a DOS batch file (.BAT) file.

Note that when you want to quit the batch page without having saved the batch file, the GUI asks 'Batch definition is changed, are you sure you want to discard the changes?' Answering 'Yes' then means that you don't want to save the batch file that you just prepared.

To execute the batch file, you can click "Run batch file" on the TOXSWA page. A DOS-box then informs you during batch execution, which of the individual runs TOXSWA is executing.

7 Execution of a TOXSWA simulation

In this chapter we describe the steps involved in running TOXSWA. It is assumed that you have already executed the trail run described in Chapter 4, and that you have already gained some experience in running the model.

Chapter 6 described the use of the Graphical User Interface for preparing the input files for TOXSWA, running TOXSWA and viewing the output of TOXSWA graphically.

The sequence of steps to be followed to run the TOXSWA program are described below.

1. Select an existing scenario or define a scenario by adapting an existing scenario, or press the "New" button and change the parameters in the pages belonging to the scenario. Save the adapted scenario with the original name("Save"), or save the scenario with a new name ("Save as").
2. Define a pesticide likewise.
3. Run TOXSWA.
4. View the exposure concentrations in the table at the *Concentration in time* page, and view the output graphically via the graphs in the GUI

First press "Run TOXSWA" button in the GUI.

A TOXSWA simulation can only be run if the nine input files described in Chapter 4 are present in the `c:\toxswa\scenarios\name_scenario` for the scenario and in `c:\toxswa\pesticides\name_pesticide` for the pesticide.

The output of the simulation is directed to the output files *.OUT in `c:\toxswa\runs\name_scenario+name_pesticide`. While the program is running, error messages are directed to the screen, and also to the file MESSAGE.OUT, which is discussed in Section 5.2.4.

While reading the input files, TOXSWA checks if the parameter values are within the proper range and reports an error when this is not the case.

When a combination of a scenario and a pesticide is executed for the first time, the DOS-box echoes:

```
Could not find
c:\toxswa\runs\name_scenario+name_pesticide\*.out
```

This message can be ignored, it does not affect the simulation.

During execution of the simulation run, the DOS-box echoes the progress of the simulation:

```
Time simulated: 0.0 d
```

The program stops immediately if the selected time step is too large compared to the defined spatial discretisation and dynamics of the simulated system (see Chapter 7 in Adriaanse, 1996). The message sent to your screen is

```
Positivity conditions wl (wb) not fulfilled
see message.out.
Program stops.
```

You will find the same message in the file MESSAGE.OUT. You should then first verify if your selected time step corresponds more or less with the estimation of a possible time step (see Section 8.2). If it does, you can continue via iteration by halving the time step and redo a simulation until the program runs.

While TOXSWA runs, two kinds of messages may be echoed to the DOS-box and to the MESSAGE.OUT file. Warning messages indicate that you should keep a particular warning in mind when interpreting the output. An error message indicates that the output of the simulation will not be valid, unless you correct the error. Annex 2 gives a list of all messages, with some advice for solutions. Note that for some messages occurring over 20 times (for some others over 50 times), they will no longer be written to the screen and the MESSAGE.OUT file, to prevent this file from becoming very large. The run may also fail without messages being given. This is the first version of the program, so its performance under varying conditions has not yet been extensively tested.

After the simulation is finished the screen echoes:

```
    end of simulation
Stop - Program terminated
```

In the directory `c:\toxswa\runs\name_scenario+name_pesticide` the output files have then been created. Examples of these output files are shown in Figures 14-26 in Chapter 5.

One simulation run with TOXSWA may take a considerable amount of time, depending on the number of segments defined, the size of the calculation time step, the total simulation time and the power of your PC (see Chapter 9). It may be worthwhile to use the batch option in the TOXSWA-GUI (see Section 6.8).

8 Estimation of input parameters

8.1 Introduction

To execute simulations with TOXSWA values for all input parameters are required. Often, not all parameters are measured or known for the simulations you wish to simulated. This chapter provides some suggestions for estimating parameters with the aid of information from other sources, or it provides some best guesses in case no information is available. The choice of a combination of time and space steps is discussed separately, because they are subject to several restrictions.

8.2 Space step and time step for water layer and sediment

This section discusses a procedure to estimate possible space and time steps to solve the mass conservation equations of the water layer and the sediment numerically. The procedure helps you to make an acceptable first guess. A full procedure going beyond a first guess, would become complicated, because it would include an iterative step, optimising the time and the space step (i.e. segment length). Another complication is that the space and time steps might not result in a stable and positive solution of the differential equations for all concentration levels. The positivity conditions depend on the concentration, because sorption has been described with the aid of a Freundlich sorption isotherm, which is non-linear. The program verifies whether the selected space and time steps are sufficiently small to fulfil the positivity conditions and to result in a positive solution of the mass conservation equations, i.e. a positive concentration. If the conditions are not met, the program stops. The MESSAGE.OUT file then shows you, which of the positivity conditions has not been fulfilled.

Below, we assume that the time and space step in the water layer are the strictest constraints for simulation in most situations, because pesticide behaviour in the water layer generally is more dynamic than that in the sediment layer. The time step in the water layer equals the time step in the sediment layer in TOXSWA 1.2.

Space step
The space step can be estimated by assuming a constant flow velocity (u) and constant water depth in the water body (assumptions in version 1.2 of TOXSWA) and a linear sorption isotherm describing sorption to suspended solids. A constant segment size ()x) is assumed for this estimation procedure. If this is not true for your simulation, use the largest segment size from your case. Assuming that the numerical dispersion E_{num} can be ignored, the maximum allowable space step is

$$\Delta x \leq \frac{E_x}{0.5u} \tag{4}$$

for TOXSWA 1.2, because it uses the explicit central difference calculation scheme (see Section 7.2.2 in Adriaanse, 1996). E_x is the longitudinal dispersion coefficient, characterising the watercourse.

Time step
We can not give an advice for the time step for an explicit central difference calculation scheme. First try the default time step of TOXSWA 1.2 (600 s). If the program runs immediately, you might retry with a doubled time step, etc., in order to find the shortest run time possible. If the program fails to run for the selected time step, look in the MESSAGE.OUT file, which of the positivity conditions has not been met. If the RBD, LBD, ROD or LOD condition are not met, you should enlarge the dispersion coefficient (if this is still realistic) or diminish the segment size. If the LDD or RDD conditions are not met the time step should be made smaller, e.g. you can halve the time step until the program runs.

8.3 Water layer

The water layer parameters, given in the WLNU.INP, WLPA.INP and WLST.INP files, are discussed in this section.

8.3.1 WLNU.INP

Numerical weight factors
The weight factors (*betawl*, *thetawl*) are fixed at 0.5 and 1.0 respectively, in TOXSWA 1.2, corresponding to an explicit central finite difference solution method. The time and space parameters are discussed in Section 8.2.

Space parameters
The length of the water body (*xdit*) depends on the water body that you want to simulate. In version 1.2 of TOXSWA the buffers are not necessary because the flow in the water body (*u*) is constant, so their lengths (*xfb*, *xeb*) have been fixed at 0.

Number of segments
The length of the water body divided by the number of segments (*nxsedit*) determines the segment size, if you distribute the segments uniformly over the total length. See Section 8.2 (space step) to find out how to select a possible segment size, i.e. space step for your case. The number of segments in the front and end buffers (*nxsefb*, *nxseeb*) have been fixed at zero in version 1.2 of TOXSWA.

Lengths of segments
Depending on your needs, the lengths of the segments can be constant over the length of the water body or their lengths can be variable. See Section 8.2 (space step) for an advice on possible lengths.

8.3.2 WLPA.INP

Concentration and organic matter content of suspended solids
The constant concentration of suspended solids (*coss*) depends much on the flow regime in the water body and the wind influence in the water layer. A concentration of 100 g m^{-3} may occur in a shallow lake after a gale. In a fast flowing water body it can even be higher. The organic matter content of suspended solids (*raomss*), if not measured, can be estimated by taking the organic matter content of the top layer of the sediment (*raomwb*, WBPA.INP).

Mass of macrophytes
A dry weight of macrophytes of 300 g m^{-2} is a realistic value for the average peak mass in Dutch ditches (Bloemendaal et al., 1988). For spring (May) average peak masses may be 50 g m^{-2}, for summer 300 g m^{-2} and for autumn (October) 150 g m^{-2}. These values are based on data from a cut-off bend of a river with a water layer of about 0.50 to 1 m. The values mentioned above can be used for water bodies with water layers of 0.50 to 1 m deep. The macrophyte mass is probably lower for a water body with a water layer of 0.25 m. Most of the macrophyte mass is located close to the water surface. We estimate that the macrophyte mass in water bodies with a water layer of 25 cm is about 2/3 of the masses mentioned above for deeper water layers (personal communication , T.C.M. Brock, SC-DLO, 1998). Therefore, in water bodies with water depths of 0.25 m we estimate 35 g m^{-2} dry weight of macrophytes for spring, 200 g m^{-2} for summer and 100 g m^{-2} for autumn to be realistic values in case of a high macrophyte densities.

An estimation of a realistic low macrophyte mass can be derived from Roelofs and Bloemendaal (1988). They found that the mass frequently is less than 100 g dry weight m^{-2} in oligotrophic surface waters with sediments with a low nutrient status. Most of this macrophyte mass resides in the roots in the sediment. Bloemendaal et al. (1988) found that mass of roots could be up to 50-80% of the total macrophyte mass. Combining the above findings, we estimate that 20-50 g dry weight m^{-2} is a realistic value for low macrophytes density occurring e.g. in oligotrophic waters with sediments having a low nutrient status. Taking the season into account, 20 g dry weight m^{-2} is an appropriate estimate for spring and autumn, and 50 g dry weight m^{-2} for summer (personal communication T.C.M. Brock, SC-DLO, 1998).

Geometry of neighbouring plot of land
The length of the draining lot (*leplot*) perpendicular to the water body located on one or both sides of the water body is a dummy value in TOXSWA 1.2. So the parameters set for upward or downward seepage are not related anymore to this parameter, like in TOXSWA 1.0.

8.3.3 WLST.INP

Initial concentrations
The total mass concentrations (*castwl*) of the pesticide have to be entered in each segment.

Constant background concentration in the air
The pesticide background concentration in the air (*coair*) has been fixed at zero in TOXSWA 1.2.

8.4 Sediment

The sediment parameters, given in the WBNU.INP, WBPA.INP and WBST.INP files, are discussed in this section.

8.4.1 WBNU.INP

Numerical weight factors
The weight factors (*betawb*, *thetawb*) have been fixed at 0.5 and 1.0 respectively, in TOXSWA 1.2, corresponding to an explicit central finite difference solution method.

Time parameters
The time step for the sediment (*deltwb*) should be set equal to the time step selected for the water layer.

Number of segments and thicknesses of segments
The segments have to be distributed over the total thickness of the sediment. The segments close to the water layer have to be much thinner. Diffusion of substance into the sediment may cause very sharp concentration fronts. To be able to simulate very sharp concentration fronts correctly, the upper segments need to be about 1 mm thick. The segment thickness may increase gradually, up to about 1 cm.

8.4.2 WBPA.INP

Physical properties of sediment
Little information on sediment properties as a function of depth is available. The bulk density (*bdwb*), porosity (*por*) and tortuosity (*tor*) given in the Dutch standard scenario may be used for a ditch in a sandy soil. They are based on bulk densities and porosities measured in the experimental ditches of SC-DLO, that are representative for ditches in a sandy area with a well-developed natural detritus layer (see Table 1).

Table 1 Bulk density and porosity as a function of depth in of the experimental ditches (personal communication, S.J.H. Crum, SC-DLO, 1996)

Layer (cm)	Bulk density (kg m^{-3})	Porosity (m^3 m^{-3})
0-1	80	0.82
1-2	220	0.77
2-4	670	0.62
4-10	1500	0.36

When the bulk density and the porosity are not available, they might be derived from the particle size distribution. Wösten (1997a, 1997b) described continuous pedotransfer functions to derive dry bulk densities and the density of the solid phase for soils as a functions of the clay and silt fractions, the organic matter content and sometimes the median sand particle size. The pedotransfer functions have been derived for well-settled, non-disturbed soils, and so the bulk densities calculated in this way may overestimate the bulk density of the sediment. The porosity of the sediment may be underestimated, in this way.

The tortuosity can be estimated by taking the results of a literature compilation of Leistra (1978) for porosities up to 0.50, as shown in Table 2. Above a porosity of 0.50, we suggest to use the value of the porosity of the segment (porosity and tortuosity are equal).

Table 2 Tortuosity for porosities up to 0.50 m^3 m^{-3} (Leistra, 1978)

Porosity (m^3 m^{-3})	Tortuosity (m^2 m^{-2})
0.10	0.03
0.20	0.10
0.30	0.20
0.40	0.34
0.50	0.50

Organic matter content

As a rule of thumb the conversion factor 0.58 is often used to convert the organic matter content into the organic carbon content (or the factor 1.7 to convert the organic carbon content into the organic matter content). However, recent research (STOWA, 1997) demonstrated that for freshwater sediments the factor of 1.7 is an underestimation and that a factor of 1.97 is a better estimation. This factor is based on linear regression between the total organic carbon (TOC) content and the loss-on-ignition of 38 Dutch freshwater sediments. Therefore, we recommend to use this factor 1.97 to convert the organic carbon content into the organic matter content.

Dispersion in sediment

The dispersion length (*ldis*) is a measure of the length over which mixing takes place. Boesten (1986) indicated that the dispersion length for solute movement in field soils under natural conditions is in the range 2 to 30 mm.

8.4.3 WBST.INP

Initial concentrations
The total mass concentrations of the pesticide have to be entered in each sediment segment.

8.5 Hydrology: HY.INP

The hydrology parameters are discussed in this section.

Flow velocity, depth of water layer and dispersion coefficient
Flow velocity (*u*) and water depth (*wdh*) largely determine the dispersion coefficient, E_x (*kds*). Relations between these parameters were developed for large water bodies like rivers. Generally, they implicitly include wind effects on dispersion as well. These relations do not explain the dispersion determined in small surface waters like ditches. Therefore, we did not implement such a relation in TOXSWA. In literature, only a few dispersion coefficients are available that have been determined in small watercourses. Table 3 presents dispersion coefficients determined in some Dutch ditches and brooks. Except the experimental ditches, the watercourses may be representative for small natural streams outside the Netherlands. The dispersion coefficients determined in the experimental ditches demonstrate that even when the flow velocity is near zero, dispersion occurs. When the flow velocity is zero, some dispersion may occur because of wind effects in longitudinal direction.

Table 3 Flow velocities, water depths and dispersion coefficients

Watercourse	Flow velocity ($m\ d^{-1}$)	Water depth (m)	Dispersion coefficient ($m^2\ d^{-1}$)	Reference
Experimental ditch	5-6	0.50	45-70	Adriaanse (Pers. com.)
Ditch Lopikerwaard polder	3950	0.16	16000	De Heer, 1979
Ditch Lopikerwaard polder	4190	0.21	5100	De Heer, 1979
Ditch Lopikerwaard polder	4640	0.18	18600	De Heer, 1979
Ditch Lopikerwaard polder	5640	0.15	6280	De Heer, 1979
Hupselse brook	5184	0.5	3456	Van Straten, 1979
Bornse brook	34560	0.3	112320	Van Straten, 1979

We found that the dispersion coefficients determined in the experimental ditches were reasonably well estimated by equation of Jain (Young and Wallis, 1993). Therefore, we recommend to use the equation of Jain for watercourses with flow velocities up to about 1000 m d^{-1}. The equation of Jain reads:

$$E_x = \beta \frac{\bar{u}^2 O^3}{kAU^*} \quad (5)$$

with

E_x	=	dispersion coefficients in the direction of flow ($m^2\ d^{-1}$)
β	=	dimensionless parameter ($\beta \leq 0.0164$, we here assumed $\beta = 0.0164$)
k	=	dimensionless transverse mixing coefficient ($k = 0.4$ for channels with small scale longitudinal non-uniformity, such as sidewall irregularities (Fischer et al., 1979))
$\bar{u}$	=	average cross-sectional flow velocity (=u in TOXSWA)
U^*	=	shear velocity ($m\ d^{-1}$) ($U^* \cong 0.1\ \bar{u}$; Lijklema and Koelmans, 1991)
O	=	width of the water surface (m)
A	=	cross sectional area of flow (m^2)

We found that the dispersion coefficients determined for the other watercourses of Table 3 were better estimated by Fischer's equation than by that of Jain. Therefore, we recommend Fischer's formula (Fischer et al., 1979) for watercourses with flow velocities above 1000 $m\ d^{-1}$:

$$E_x = 0.011 \frac{\bar{u}^2 O^2}{hU^*} \quad (6)$$

with

h	=	water depth in the watercourse (m)

Temperature
The average temperature (T) of the system (water layer and sediment) has to be entered.

Seepage and concentration in seepage
When water from the neighbouring lot enters the water body there is upward seepage through the bottom, i.e. a negative seepage flux. When water infiltrates from the water body into the neighbouring field lot there is downward seepage through the bottom, i.e. a positive seepage flux. The pesticide concentrations in the water entering the water body have to be estimated or calculated, e.g. by estimating the concentration leaching from the neighbouring soil with the aid of a leaching model .

8.6 Loadings: SL.INP

The substance loading parameters are discussed in this section.

Number of loadings
The number of loadings has to be entered.

Time, mass and stretch of water body
The times of loading should be entered in chronological order. The mass deposited per square metre water surface area (g m^{-2}) from e.g. a spray drift event can be calculated by multiplying the field dose (g m^{-2}) with the drift fraction (-). Note that the dose in e.g. kg ha^{-1} and the drift percentage in % have to adapted to the proper dimensions (!).

You can simulate a point source release into the water body by allowing the pesticide mass to enter one (small) water body segment. To simulate e.g. drift deposition on the entire water body or a large section of the water body the pesticide mass should enter the water body over the wished stretch of the water body, which is composed of several or many water body segments.

8.7 Substance: SU.INP

The pesticide parameters are discussed in this section. Some parameter values for pesticides are systematically presented in the Pesticide Manual (Tomlin, 1994). The properties that are provided include: molecular mass, saturated vapour pressure, solubility, sorption coefficient to soil and half-life in water and soil.

Transformation in water layer and sediment
The transformation half-life should be based on site-specific data, when simulations are compared with field measurements. For the purpose of ranking pesticides values from literature can be used (e.g. Tomlin 1994). Often, transformation half-lives have been determined in water-sediment studies. For a large number of pesticides transformation half-lives are listed by Linders et al. (1994). TOXSWA needs individual half-lives characterising transformation (and not decline!) in the water and sediment layers. A Dutch Workgroup currently studies how to determine best the individual half-lives from the reported standard water-sediment studies. First results including a preliminary procedure are expected to become available by 1 January 2000. Now, we suggest to use the half-life of the entire water-sediment system for both the water layer and the sediment.

The half-life at 20 °C should be entered. When the half-life has been measured at another temperature, it should be corrected to the half-life at 20 °C with Eq. (1) in Section 2.5 and the molar Arrhenius activation energy.

Molar Arrhenius activation energy
For about 50 experiments covering a range of pesticides and soils the FOCUS Soil Modelling Workgroup (1997) found the average value of the molar Arrhenius activation energy to be 55 kJ mol^{-1} (S.D. 15 kJ mol^{-1}). The range of activation energies was from 20 to 100 kJ mol^{-1}. The value 55 kJ mol^{-1} can be used as default value.

Note that all values of the molar activation energy E were determined for soils. In surface waters additional processes as photolysis may occur, and in sediments

anaerobic conditions may affect microbial transformation. So, Eq. (1) might not be well applicable in surface water. Further research is needed on the temperature dependency of transformation in water and sediment.

Sorption to macrophytes
Coefficients of sorption to macrophytes are hardly available. The sorption of nine pesticides to the aquatic macrophytes *Chara globularis*, *Elodea nuttallii* and *Lemna gibba* was studied by Crum et al. (1999). The sorption isotherms for compounds, not being herbicides were found to be almost linear (Freundlich exponent: 0.9-1.1). For the herbicides atrazine and linuron sorption was found to depend strongly on the concentration of the herbicide in the water phase. The macrophytes were affected by the herbicides, especially when concentrations became higher. A reasonable correlation (R^2 = 0.81) was found for the relation

$$\log K_d = 3.2 - 0.65 \log c_{sol} \quad (7)$$

between the sorption coefficient (K_d) of pesticides (excluding herbicides) and their solubility in water (c_{sol}). The equation:

can be used for a first estimate of the sorption coefficient of a pesticide to aquatic

$$\log K_{om} = 3.37 - 0.64 \log c_{sol} \quad (8)$$

macrophytes. Or when the organic matter content of the macrophytes is known:

If more accurate information on pesticide sorption to specific macrophytes is required, the sorption should be measured.

Sorption to suspended solids and sediment organic matter
The sorption coefficient based on the organic matter content K_{om} can be derived from the sorption coefficient based on the organic carbon content K_{oc} by multiplying the K_{oc} with the factor 1.7 or 1.97 (see explanation under *organic matter content* in Section 8.4). When no sorption coefficient is available for suspended solids or sediment organic matter, the sorption coefficient based on soil organic matter studies can be used. A compilation of 243 soil K_{om} values has been reported by Linders et al. (1994).

Volatilization
According to Liss and Slater (1974), exchange coefficients of the pesticide in air (k_g) and water (k_l) can be derived, from

$$k_l = k_{l,CO_2} \frac{\sqrt{M_{CO_2}}}{\sqrt{M_{substance}}} \quad (9)$$

$$k_g = k_{g,H_2O} \frac{\sqrt{M_{H_2O}}}{\sqrt{M_{substance}}} \quad (10)$$

where

$k_{l,\,CO2}$	exchange coefficient of CO_2 in the liquid phase (Liss and Slater estimated a $k_{l,CO2}$ of 4.8 m d^{-1});
M_x	molecular weight of substance x (M_{CO2} = 44 g mol^{-1}; M_{H2O} = 18 g mol^{-1});
$k_{g,H2O}$	exchange coefficient of H_2O in the vapour phase (Liss and Slater estimated a $k_{l,H2O}$ of 720 m d^{-1}).

The Henry coefficient depends on the temperature (Adriaanse, 1996). It is calculated in TOXSWA using the saturated vapour pressure (P) and the solubility of the pesticide (c_{sol}). The temperatures at which they were measured have to be entered. Tomlin (1994) and Hornsby et al. (1996) list molecular masses, saturated vapour pressures and solubilities for most pesticides.

The enthalpy of vaporization depends on the substance. Smit et al. (1997) estimated an average enthalpy of vaporization of 95 kJ mol^{-1} from literature data of 16 pesticides (range: 58 to 146 kJ mol^{-1}) . The saturated vapour pressure is a basic physical property of the substance, hence the average estimated by Smit et al. (1997) is valid for surface water as well. We suggest to use 95 kJ mol^{-1} as the default value, when no other value is available.

The enthalpy of dissolution depends on the substance. For most pesticides a enthalpy of dissolution of 27 kJ mol^{-1} can be taken as default value (see Bowman and Sans, 1985; range was -17 to 156 kJ mol^{-1}).

Exchange between water layer and sediment
The diffusion coefficient in water (D_w) may be estimated from the molecular structure of the pesticide using the Hayduk and Laudy method described by Lyman et al. (1982). The value of D_w for molecules with a molecular mass of about 200 will usually be about 0.4 cm^2 d^{-1} (Jury et al., 1983; Westein et al., 1998). Usually the output of TOXSWA is not sensitive to the diffusion coefficient, so its estimation is not crucial.

9 The TOXSWA 1.2 software

9.1 Hardware and software requirements

Operating TOXSWA requires an IBM-compatible personal computer with at least a 486 processor and about 5 Mb of free space on the hard disk. Operating the TOXSWA Graphical User Interface requires at least 4 Mb RAM hardware, and Windows95 installed on your computer.

TOXSWA 1.2 has been developed in FORTRAN-77 with Digital Visual Fortran version 5.0, using Microsoft's Developer Studio97. The 32-bits executable has been compiled and linked with Digital Visual Fortran. Because of the portability of FORTRAN it can be compiled on different platforms, including VMS.

Linked to the TOXSWA program is the FORTRAN library TTUTIL, consisting of frequently used standard routines, for instance file handling (open, close, write, read, etc.) and input range checking (Rappoldt and Van Kraalingen, 1990).

The TOXSWA Graphical User Interface described in Chapter 6 and running under Windows95/NT was developed using Delphi 4 by Borland International[3].

Simulation of the example input that is provided with TOXSWA 1.2 takes about 8 minutes on a Pentium II 400 MHz PC.

9.2 Installation of TOXSWA on your computer

A ZIP file containing TOXSWA 1.2 can be downloaded from the SC-DLO internet site www.sc.dlo.nl. After downloading the ZIP file, extract the ZIP file to a temporary directory (e.g. `c:\tmp`). Next, run the `SETUP.EXE` file by double clicking `SETUP.EXE` in the temporary directory (`c:\tmp\SETUP.EXE`). Then, a sequence of windows will appear on the screen guiding you in the further installation procedure. Note that if you install the TOXSWA software not in the suggested directory c:\toxswa the Graphical User Interface will not work properly.

After installation the following (sub)directories have been created:

```
c:\toxswa
c:\toxswa\gui
c:\toxswa\pesticides
c:\toxswa\pesticides\cpf
c:\toxswa\scenarios
```

[3] Note that in some countries communication between TOXSWA and the GUI can be troubled, because the number formats do not match. This problem can be solved by changing the Regional settings of the computer. Click -My Computer -Control Panel - Regional settings, and select English.

```
c:\toxswa\scenarios\NLstandard_AU
c:\toxswa\scenarios\NLstandard_SP
c:\toxswa\source
```

The `toxswa` directory contains the executable `TOXSWA_12.EXE` and the `readme.txt` and `install.txt` files, which provide information about the TOXSWA software and the installation procedure. The `gui` directory contains the files of the graphical user interface. The `cpf` subdirectory contains the input file of the example pesticide chlorpyrifos. The `NLstandard_AU` and the `NLstandard_SP` subdirectories contain the input files of the Dutch standard scenarios for autumn and spring, respectively. Finally, the `source` directory contains the files with the source code of TOXSWA.

For use of TOXSWA, it is convenient to make a shortcut from the file `toxswaGUI.exe` to your computer desktop.

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Annexes

Annex 1 Input variables

Legend

Variable type

C = character string
I = integer
R = real

Page from TOXSWA GUI

Scenario
W = water body
H = hydrology
I = initialisation
M = simulation
O = output

Pesticide
T = transformation
S = sorption
V = volatilization
L = loading

TOXSWA input file

Files = files.inp
wlnu = wlnu.inp
wlpa = wlpa.inp
wlst = wlst.inp
wbnu = wbnu.inp
wbpa = wbpa.inp
wbst = wbst.inp
hy = hy.inp
opout = opout.inp
su = su.inp
sl = sl.inp

The parameters in the table are the names of parameters in the conceptual model in Adriaanse (1996) or in model extensions described in Chapter 2 of this report. The units in the table concern the units in the input files. The units in the Graphical User Interface may differ for some parameters.

Variable	Type	Page	File	Parameter	Meaning	Units
aetf	R	T	su	E	molar Arrhenius activation energy for transformation	J/mol
betawb	R	-	wbnu	β	numerical weight factor for space	-
bdwb(1-*nzsewb*)	R	W	wbpa	ρ_b	bulk density dry sediment material	kg/m^3
betawl	R	-	wlnu	β	numerical weight factor for space	-
castwb(1-*nzsetot*)	R	I	wbst	$c^{\wedge *}$	initial (start) mass concentration pesticide in sediment	g/m^3
castwl(1-*nxsetot*)	R	I	wlst	$c^{\wedge *}$	initial (start) mass concentration pesticide in water layer	g/m^3
coair	R	-	wlst	c_a	constant background concentration pesticide in air	g/m^3
colot	R	H	hy		concentration of pesticide in seepage water	g/m^3

coobkomss	R	S	su	$c_{e,ss}$	concentration of pesticide at which $K_{om,ss}$ of the suspended solids has been observed	kg/m^3
coobkomwb	R	S	su	$c_{e,wb}$	concentration of pesticide at which the K_{om} of the sediment material has been observed	kg/m^3
cosol	R	V	su	c_{sol}	solubility of pesticide in water	g/m^3
coss	R	W	wlpa	*ss*	concentration suspended solids	g/m^3
deltout	R	M	opout		time step for output	d
deltwb	R	-	wbnu		simulation time step sediment	s
deltwl	R	M	wlnu		simulation time step water layer	s
dt50wb	R	T	su		transformation half-life sediment	d
dt50wl	R	T	su		transformation half-life water	d
dwmp	R	W	wlpa	*DW*	dry weight macrophytes per m^2 bottom	g/m^2
enxslus	R	L	sl		end of stretch onto which spray drift loading is deposited	m
exfrss	R	S	su	n_{ss}	Freundlich exponent for sorption to suspended solids	-
exfrwb	R	S	su	n_{wb}	Freundlich exponent for sorption to sediment material	-
hyinp	C	F	files		path and name of file HY.INP	-
iwbsy	I	M	opout		segment number in water layer at/under which output is desired	-
kdfw	R	V	su	D_w	diffusion coefficient of pesticide in water	mm^2/d
kdmpdit	R	S	su	K_{mp}	slope of sorption isotherm based on dry weight of macrophytes	m^3/kg
kdomwb1	R	S	su	$K_{om,wb}$	sorption coefficient based on organic matter content of sediment material	m^3/kg
kdomssdit	R	S	su	$K_{om,ss}$	sorption coefficient based on organic matter content	m^3/kg
kds	R	H	hy	E_x	dispersion coefficient in water	m^2/d
kga	R	V	su	k_g	transport coefficient of pesticide in gas phase	m/d
klq	R	V	su	k_l	transport coefficient pesticide in liquid phase	m/d
ktop	I	W	opout		number of upper segments forming the top layer for which the accumulated pesticide mass will be calculated	-
ldis	R	H	wbpa	L_{dis}	dispersion length in sediment	m
leplot	R	-	wlpa	*P*	length of draining plot, perpendicular to water body and located on one or both sides,	m
lesedit	R	W	wlnu		lengths of segments in water body	m
leseeb	R	-	wlnu		lengths of segments in end buffer	m
lesefb	R	-	wlnu		lengths of segments in front buffer	m
leseebb	R	W	wbnu		lengths of segments in end buffer	m
lesewb	R	W	wbnu		lengths of segments in sediment	m
mepsat	R	V	su	ΔH_P	molar enthalpy of vaporization	J/mol
mesolt	R	V	su	ΔH_{sol}	molar enthalpy of dissolution	J/mol
mamol	R	V	su	*M*	molecular mass of pesticide	g/mol
mslus	R	L	sl		mass of spray drift loading	g/m^2
ntslus	I	L	sl		number of spray drift loadings	-
nwbsy	I	-	opout		number of sediment subsystems for which output is desired	-
nxsedit	I	W	wlnu		number of segments in water body	-
nxseeb	I	-	wlnu		number of segments in end buffer wl	-
nxsefb	I	-	wlnu		number of segments in front buffer wl	-
nzseebb	I	-	wbnu		number of segments in end buffer sedim.	-
nzsewb	I	W	wbnu		number of segments in sediment	-
opoutinp	C	-	files		path and name of file opout.inp	-

op_ecsegmentnr	I	O	opout		output file ECxxx.OUT (exposure concentrations in wl+wb at segment wl) desired	-
op_dbdit	I	O	opout		output file DBDIT.OUT (distribution substance in total water body) desired	-
op_dbsegmentnr	I	O	opout		output file DBxxx.OUT (distribution substance in wl+wb at segment wl) desired	-
op_icwb	I	O	opout		output file ICWB.OUT (initial calculations for sediment) desired	-
op_icwlhy	I	O	opout		output file ICWLHY.OUT (initial calculations for water layer and hydrology) desired	-
op_input	I	O	opout		output file INPUT.OUT (echo of all input) desired	-
op_slmd	I	L	sl		option model specified input drainage	-
op_slmr	I	L	sl		option model specified input runoff	-
op_slud	I	L	sl		option user specified input drainage	-
op_slur	I	L	sl		option user specified input runoff	-
op_slus	I	L	sl		option user specified input spray drift	-
op_wbmbsegmentnr	I	O	opout		output file WBMBxxx.OUT (mass balance for sediment sub-system) desired	-
op_wbscosegmentnr	I	O	opout		output file WBSCOxxx.OUT (concentrations in sediment subsystem) desired	-
op_wbmball	I	O	opout		output file WBMBALL.OUT (mass balance for all sediment sub-systems) desired	-
op_wlmb	I	O	opout		output file WLMB.OUT (mass balance water layer) desired	-
op_wlmbsegmentnr	I	O	opout		output file WLMBxxx.OUT (mass balance segment water layer) desired	-
por(1-*nzsewb*)	R	W	wbpa	,	porosity (volume fraction of void water) (as a function of depth, end buffer excluded)	-
psat	R	V	su	*P*	saturated vapour pressure of pesticide	Pa
qseif	R	H	hy	*q*	seepage	$m^3/m^2.d$
raomss	R	W	wlpa	$m_{om,ss}$	mass ratio of organic matter of suspended solids	-
raomwb	R	W	wbpa	$m_{om,wb}$	mass ratio of organic matter in dry sediment material	-
sisl	R	W	wlpa	s_1	side slope water body, horizontal/vertical	-
slinp	C	-	files		path and name of file SL.INP	-
stxslus	R	L	sl		start of stretch onto which spray drift loading is deposited	m
suinp	C	-	files		path and name of file SU.INP	-
te	R	H	su	*T*	temperature	K
tepsat	R	V	su		temperature at which saturated vapour pressure was measured	K
tesol	R	V	su		temperature at which solubility pressure was measured	K
thetawb	R	-	wbnu	2	numerical weight factor for time	-
thetawl	R	-	wlnu	2	numerical weight factor for time	-
tor(1-*nzsewb*)	R	W	wbpa	8	tortuosity	-
tslus	R	L	sl		time of spray drift loading	d
ttot	R	M	wlnu		total simulation time	d
u	R	H	hy	*u*	constant flow velocity in water body	m/d
wbnuinp	C	-	files		path and name of file WBNU.INP	-
wbpainp	C	-	files		path and name of file WBPA.INP	-
wbstinp	C	-	files		path and name of file WBST.INP	-

wdh	R	H	hy	*h*	constant water depth in water body	m
wdhfl	R	W	wlpa	h_w	water depth defining perimeter for sediment	m
wibot	R	W	wlpa	*b*	bottom width of water body	m
wlnuinp	C	-	files		path and name of file WLNU.INP	-
wlpainp	C	-	files		path and name of file WLPA.INP	-
wlstinp	C	-	files		path and name of file WLST.INP	-
xdit	R	W	wlnu		total length of water body	m
xeb	R	-	wlnu		length of end buffer water body	m
xfb	R	-	wlnu		length of front buffer water body	m
zebb	R	W	wbnu		length of end buffer sediment	m
zwb	R	W	wbnu		length of sediment	m

Annex 2 Error messages

This annex lists all possible warning and error messages. Most messages are self-evident and not further explained here. If messages concerning mass balances occur over 20 times they are no longer written to the screen and MESSAGE.OUT, in order to prevent the MESSAGE.OUT file from becoming extremely large. If messages concerning the positivity conditions occur over 50 times, they are no longer written to the MESSAGE.OUT file for the same reason.

A.2.1 Warnings and errors on screen

```
Warning:
More than 0.1% mass missing in
mass balance water layer;
see message.out

Error:
Positivity conditions wl not fulfilled;
see message.out
Program stops

Error:
Never ending loop in wlso;
see message.out
Program stops

Error:
Positivity conditions wb not fulfilled;
see message.out
program stops

Warning:
More than 0.1% mass missing in
mass balance of one sediment subsystem;
see message.out

Error in wbnu.inp:
Deltwb should be equal to deltwl in TOXSWA 1.2
Programs stops
```

A.2.2 Warnings and errors in MESSAGE.OUT

A.2.2.1 Input

```
Error in input wlnu.inp,
actual length array lesefb is not equal
to declared length, please correct data
```

```
Error in input wlnu.inp,
actual length array lesedit is not equal
to declared length, please correct data

Error in input wlnu.inp,
cumulative length of segments in water body is not equal
to declared length, please correct data

Error in input wlnu.inp,
actual length array leseeb is not equal
to declared length, please correct data

Error in input wlst.inp,
actual length array castwl is not equal
to declared length, please correct data

Error in wbnu.inp:
deltwb should be equal to deltwl in TOXSWA 1.2 !
Program stops

Error in input wbnu.inp,
actual length array lesewb is not equal
to declared length, please correct data

Error in input wbnu.inp,
cumulative length of segments in sediment is not equal
to declared length, difference is .... m
please correct data

Error in input wbnu.inp,
actual length array leseebb is not equal
to declared length, please correct data

Error in input wbpa.inp,
actual length array bdwb, por or tor is not equal
to declared length, please correct data

Error in input wbpa.inp,
actual length array raomwb is not equal
to declared length, please correct data

Error in input wbst.inp,
actual length array castwb is not equal
to declared length, please correct data

Error in input opout.inp,
actual length array iwbsy is not equal
to declared length, please correct data

Error in input wlnu.inp,
multiple of simulation timestep deltwl
is not equal to one day (86400 s)
```

```
Warning: timestep for output (deltout) is not
a multiple of calculation timestep deltwl
therefore deltout = .... d is replaced by
deltout = .... d

Warning:
number of segments for average concentration in top
sediment ktop is greater than total number of
sediment segments
ktop is corrected from .... to .... segments

Warning: input time for ....
(loading no ....)
is not a multiple of calculation timestep
therefore input time .... d
is replaced by .... d

Warning: input distance for ....
(segment ....)
matches not with defined segment lengths, therefore
input distance .... m is replaced
by … m

Error in input sl.inp,
actual length array tslus, mslus, stxslus or enxslus
is not equal to declared length, please correct data

Error in input sl.inp,
loading from spray drift no .... and no ....
concur

Error in input sl.inp,
loadings from spray drift not entered in
chronological order, please change order

Warning:
substance present in water layer and loading of
substance taking place simultaneously at start
of simulation
```

A.2.2.2 Mass balances

```
Warning: .... % of initial and loadings plus
Accumulated mass incoming from sediment is
missing in the mass balance of the water layer
at time step .... ( .... day)
qumwl = .... g and
totmwlst-cuinwb = .... g
See output in wlmb.out
```

If this message is repeated many times, and deviations from the mass balance exceed 0.1% considerably, the results of the simulation have to be analysed critically. If this message is given in the initial stage of the simulation period and the concentrations are very small (check this!), it is a numerical artefact in calculation of the mass balances.

```
Message from subroutine wbso:
More than .... iteration loops will be needed to calculate
clbj+1
for gridpoint: .... at time step: ....
in the sediment subsystem
under segment water layer: ....
Iteration values oldcowbjp1 and cowbjp1 are: ...., ....
Never ending loop !
```

See comment above.

```
Message from subroutine wbso:
Negative concentration in sediment !
at time step: .... and segment: ....
in sediment subsystem under node wl: ....
Concentration is: ....
```

See comment above.

```
Warning: Phenomenon of dispersion flux cancelling out
/exceeding advection flux would occur in sediment. (This has
been avoided with aid sofdfactors.)
Number of ocurrence of this phenomenon: ....
Time step: .... under water layer segment: ....
sediment node: ....
sofdfactormh: ....
sofdfactorph: ....
```

The combined material flux resulting from advection and its ensuing dispersion (calculated with the aid of concentration gradients) may have different directions if very sharp concentration fronts occur. The program was adjusted to solve this problem. When the number of occurrences is high, you should keep this in mind when interpreting pesticide fate in the sediment.