# Hydrodynamic Modelling with Soil and Water Assessment Tool (SWAT) for Predicting Dynamic Behaviour of Pesticides

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**Abstract** The first step in the dynamic modelling of pesticides is a reliable hydrodynamic model. SWAT (Soil and Water Assessment Tool) calculates both the dynamic hydrological response and the associated diffuse pesticide supply towards surface waters. In this study, we focus on the hydrodynamic part. First, an intensive data collection for the Nil-catchment was performed. During model set-up, a reduction of the number of model parameters was obtained using an LH-OAT sensitivity analysis. Next, the selected parameters were optimised by a manual and an auto-calibration. The auto-calibration procedure is based on a multi-objective function which incorporates the algorithms of the Shuffled Complex Evolution Method. Results of the manual and the auto-calibration are compared.

**Keywords** Hydrodynamic modelling, SWAT, sensitivity analysis, auto-calibration, pesticides

## Introduction

Dynamic models form suitable instruments for risk assessment of toxic components in natural river systems (Deksissa and Vanrolleghem, 2001). By using exposure models under time-varying conditions, risks can be determined more realistically as compared to a steady state or a static approach (Verdonck *et al*., 2002). Advantages consist in better predictions of impacts of accidental discharges, of effects of specific climatological or seasonal variations and of evolutions in water quality. A prominent example is the dynamic modelling of pesticides.

The first step in the development of a dynamic exposure model is a reliable hydrodynamic model. The hydrodynamics of a river catchment will determine to a great extent the transport of solutes, suspended sediments and colloids in the water system. SWAT was found to be the most suitable tool for modelling non-point source pollution on catchment scale. By using the SWAT model, not only hydrodynamic predictions but also predictions of pesticide loads at different parts of the river at any time can be made. In this research, SWAT is used to model the hydrodynamic behaviour of a small river called the ‘Nil’.

## Methods

### Catchment area

We focus on the Nil, a small, hilly basin situated in the French speaking part of Belgium. It drains an area of 32 km², is 14 km long and has a retention time of about 1 day. The area consists predominantly of loamy soils, 7% of the area is inhabited and the main crops grown are winter wheat (22% of the catchment area), corn (15%) and sugar beet (10%). 18% of the catchment consists of pasture. The Nil catchment was selected because it is a well documented basin, studied in detail in terms of pesticide application (Beernaerts *et al*., 2002).

### Model description

SWAT2000- the Soil and Water Assessment Tool- is developed by the USDA to predict the impact of land management practices on water, sediment and amount of chemicals originating from agriculture, in large complex river basins with varying soils, land use and management conditions over a long period of time. It is a partly physically-based and partly distributed, continuous model with a daily calculation time step (Neitsch *et al*., 2002).

In the present study, only hydrological processes are considered. The water quantity processes simulated by SWAT include precipitation, evapotranspiration, surface run-off, lateral subsurface flow, ground water flow and river flow.

We used the AVSWAT version of the model, where the simulator is integrated in a GIS by an ArcView pre-processor (Di Luzio *et al*., 2002). It uses gridded DEM data, polygon coverage's of soils and land use, and point coverage's of weather stations as basic input to the model (Figure 1).

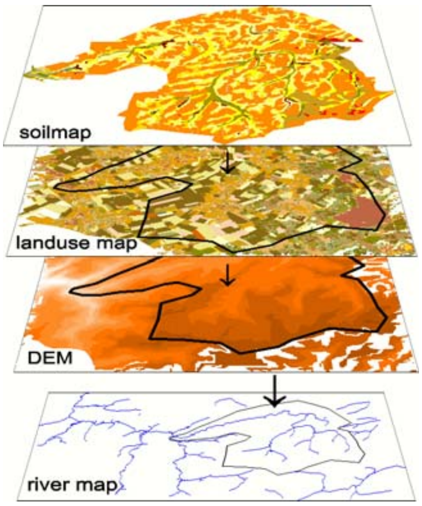


**Figure 1** Overlaying of different maps within the SWAT-model

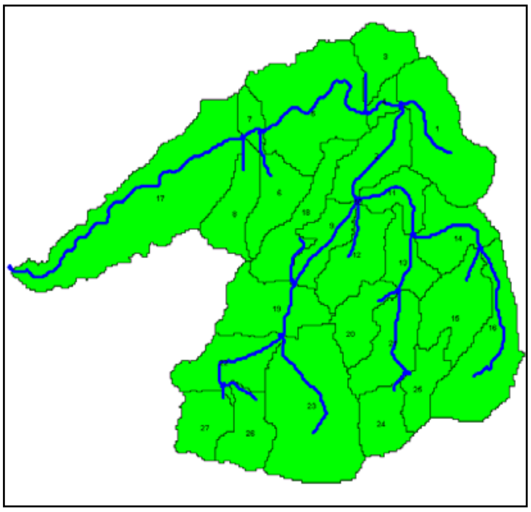

**Figure 2** Sub-basin delineation in the Nil-catchment, automated by means of a DEM

Within SWAT, a watershed is partitioned into a number of sub-basins (Figure 2), based on the threshold area which defines the minimum drainage area required to form the origin of a stream. Within the sub-basins, hydrologic response units (HRU's) are defined, which are lumped land areas consisting of unique combinations of land cover, soil and management (Neitsch *et al*., 2002).

## Input data

For the Nil-catchment, weather data from 1998 to 2002 were obtained from the Belgian Royal Meteorological Institute for the stations of Chastre and Ernage. These data include daily precipitation and daily maximum and minimum temperatures.

A DEM created by local government authorities and a 1999 land use map (Landsat) were added to the SWAT model.

A detailed soil map was created by digitizing the required parts of the maps 117E, 130E and 130W; all at scale 1:25.000 (IRSIA, 1961). The basic soil properties (percentage of sand, clay and silt; the texture class, the percentage of carbon and the horizon thickness) were obtained from the analytical database AARDEWERK (Van Orshoven *et al.*, 1993). In order to calculate the hydraulic conductivity ($K_{sat}$), pedotransfer functions from the HYPRES data base were used (Wösten *et al.*, 1998). The available water capacity (AWC) was estimated from water contents at pF 4.2 and 2.5 using the RETC-program (van Genuchten *et al.*, 1991).

For the simulation, the Nil was divided into 27 sub-basins and reaches. The sub-basins are further divided into 227 HRU's, as defined by land use and soil type.

## Sensitivity analysis and calibration

A complex hydrologic model is generally characterised by a multitude of parameters. Due to spatial variability, measurement error, incompleteness in description of both the elements and processes present in the system, etc., the values of many of these parameters will not be exactly known. Therefore, to achieve a good fit between simulated and measured data, models need to be conditioned to match reality by optimising their internal parameters.

The model calibration procedure can be either manual or automated. A manual calibration depends on the knowledge, experience and patience of the modeller and can be very time-consuming.Therefore, it is advisable to be supported by statistical techniques such as sensitivity analysis and auto-calibration. A parameter sensitivity analysis provides insights on which parameters contribute most to the output variance due to input variability. Based on this information, a calibration can be performed for a limited number of sensitive parameters.

### *The LH-OAT sensitivity analysis*

The LH-OAT method combines the OATdesign and Latin Hypercube sampling by taking the Latin Hypercube samples as initial points for an OAT-design (Figure 3) (van Griensven *et al.*, 2004).

Latin-Hypercube sampling (McKay, 1988) is a sophisticated way to perform random sampling such as Monte-Carlo sampling which results in a robust analysis requiring not too many runs. It subdivides the distribution of each parameter into N ranges, each with a probability of occurrence equal to 1/N. Random values of the parameters are generated, such that each range is sampled only once. For each of the N random combinations of the parameters the model is then run.

In the OAT (One-factor-At-a-Time) design (Morris, 1991), only one input parameter is modified between two successive runs of the model. Therefore, the changes in the output in each model run can be unambiguously attributed to the input changed in such a simulation. Considering $n$ parameters, the experiment involves performing $n$+1 model runs to obtain one partial effect for each parameter. As the influence of a parameter may depend on the values chosen for the remaining parameters, the experiment has to be repeated for several sets of input parameters. The final effect will then be calculated as the average of a set of partial effects.

As a result, the LH-OAT sensitivity analysis method is a robust and efficient method: for *m* intervals in the LH-method, a total of $m \times (n+1)$ runs is required. The LH-OAT provides ranking of parameter sensitivity (van Griensven *et al.*, 2004).

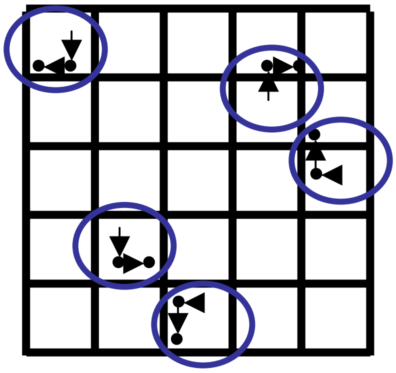


**Figure 3** Illustration of LH-OAT sampling of values for a two parameters model where X represent the Monte-Carlo points and • the OAT points (van Griensven *et al*., 2004).

### *Auto-calibration*

The auto-calibration operates by the minimisation of an objective function with the ParaSol program. ParaSol (Parameter Solutions) (van Griensven and Meixner, 2004) is a modified version of the Shuffled complex evolution algorithm (Duan et al., 1992) that allows multi-objective optimisation.

*Shuffled complex evolution algorithm (SCE-UA)*: The SCE-UA algorithm is a global search algorithm for the minimisation of a single function for up to 16 parameters (Duan et al., 1992). The SCE-UA combines several strategies and searches over the whole parameter space, hereby avoiding local optima. In a first step (zero-loop), SCE-UA selects an initial 'population' by random sampling throughout the feasible parameter space for p parameters to be optimised (delineated by given parameter ranges). The population is portioned into several "complexes" that consist of 2p+1 points. Each complex evolves independently using the simplex algorithm. The complexes are periodically shuffled to form new complexes in order to share the gained information. It has been widely used in watershed model calibration and other areas of hydrology such as soil erosion, subsurface hydrology, remote sensing and land surface modelling (Duan, 2003; Duan *et al.*, 1992) and was applied as well with success to SWAT (Eckhardt and Arnold, 2001; van Griensven and Bauwens, 2003).

*Objective function (OF)*: This objective function is similar to the Mean Square Error method (MSE) and aims at estimating the matching of a simulated series to a measured time series:

$$OF = \sum_{n=1,N} \left[ h(x_{n,measured}) - h(x_{n,simulated}) \right]^2 \qquad (1)$$

with $N$ the number of pairs of measured ($x_{measured}$) and simulated ($x_{simulated}$) variables and $h(.)$ stands for the option to apply a transformation function (such as lognormal or root function).

*Multi-objective optimisation*

Several OF's can be combined to a Global Optimisation Criterion (GOC) using (van Griensven and Meixner, 2004):

$$GOC = \sum_{m=1}^{M} \frac{OF_m * N_m}{OF_{m,\min}} \quad (2)$$

where $N_m$ is the number of observation and $OF_{m,min}$ is the minimum value for the m-th OF.

## Results and discussion

### Sensitivity analysis

The sensitivity analysis presented here only focuses on the parameters related to the hydrologic processes. The changing of the distributed parameters was performed in a lumped way by sampling a relative change (in percentage). The analysis was carried out, based on simulations for hydrology at the mouth of the river, for the period from 1998 until 2001. Results of the sensitivity analysis are shown in Table 1. This table represents the sensitivity rank of the 27 observed parameters, both for the performance for flow (OF), as for the total mass balance of the model output (MB). The former is using Eq.1 with no application of a transformation function for daily flow observations. The latter is assessed for the total amount of water that leaves the catchment at the outlet over the model period and is typically used for catchment management.

**Table 1** Parameters and parameter range used in sensitivity analysis + sensitivity ranking (with Gw. = groundwater, Evap. = evaporation, Geom. = Geomorphology) (*relative percent change)

| Name | min | max | Definition | Process | OF | MB |
|---|---|---|---|---|---|---|
| CN2 | -50 | 50 | SCS runoff curve number for moisture condition II * | Runoff | 1 | 1 |
| surlag | 0 | 10 | Surface runoff lag coefficient | Runoff | 2 | 19 |
| SMTMP | 0 | 5 | Snow melt base temperature (°C) | Snow | 3 | 13 |
| SMFMX | 0 | 10 | Maximum melt rate for snow (mm/°C/day) | Snow | 4 | 10 |
| rchrg_dp | 0 | 1 | Groundwater recharge to deep aquifer (fract) | | 5 | 2 |
| GWQMN | 0 | 1000 | Threshold depth of water in the shallow aquifer required for return flow to occur (mm) | Soil | 6 | 3 |
| sol_z | -50 | 50 | Soil depth * | Soil | 7 | 5 |
| GW_DELAY | 0 | 100 | Groundwater delay (days) | Gw. | 8 | 9 |
| SOL_AWC | -50 | 50 | Available water capacity of soil layer (mm/mm soil) | Soil | 9 | 6 |
| TIMP | 0.01 | 1 | Snow pack temperature lag factor | Snow | 10 | 16 |
| ESCO | 0 | 1 | Plant evaporation compensation factor | Evap. | 11 | 4 |
| SFTMP | 0 | 5 | Snowfall temperature (°C) | Snow | 12 | 11 |

| | | | | | | |
|---|---|---|---|---|---|---|
| SLSUBBSN | -50 | 50 | Average slope length (m/m) * | Geom. | 13 | 22 |
| GW_REVAP | 0.02 | 0.2 | Groundwater “revap” coefficient | Gw. | 14 | 8 |
| CH_K2 | 0 | 150 | Effective hydraulic conductivity in main channel alluvium (mm/hr) | Channel | 15 | 20 |
| canmx | 0 | 10 | Maximum canopy index | Runoff | 16 | 12 |
| REVAPMN | 0 | 500 | Threshold depth of water in the shallow aquifer for “revap” to occur (mm) | Gw. | 17 | 7 |
| SLOPE | -50 | 50 | Average slope steepness (m/m) * | Geom. | 18 | 21 |
| SMFMN | 0 | 10 | Minimum melt rate for snow (mm/°C/day) | Snow | 19 | 18 |
| ALPHA_BF | 0 | 1 | Baseflow alpha factor (days) | Gw. | 20 | 15 |
| BIOMIX | 0 | 1 | Biological mixing efficiency | Soil | 21 | 14 |
| ch_n | -20 | 20 | Manning coefficient for channel | Channel | 22 | 24 |
| sol_k | -50 | 50 | Soil conductivity (mm/hr) * | Soil | 23 | 17 |
| sol_alb | 0 | 1 | Moist soil albedo | Soil | 24 | 23 |
| epco | -50 | 50 | Plant evaporation compensation factor * | Evap. | 25 | 25 |
| TLAPS | -50 | 50 | Temperature laps rate (°C/km) * | Geom. | 26 | 27 |
| blai | -50 | 50 | Leaf area index for crop * | Crop | 27 | 26 |

The results for model output (MB) somehow follow those for model performance (OF). In both cases the curve number (CN2) is the most important parameter, followed by the parameters rchrg_dp and GWQMN. The importance of the groundwater parameters is not surprising, due to the fact that drainage to deeper groundwater is high. Groundwater of the Nil-catchment passes towards the adjacent river the Train. This is explained in detail below.

## Calibration

In the manual calibration, parameters influencing baseflow and surface flow are optimised. As the parameters SOL_AWC and sol_z are supposed to be determined precisely, no optimisation was performed for them. The parameters that are given priority in the auto-optimisation, are indicated with a grey background in Table 1.

The results of the manual calibration are given in Figure 4a and 4b.

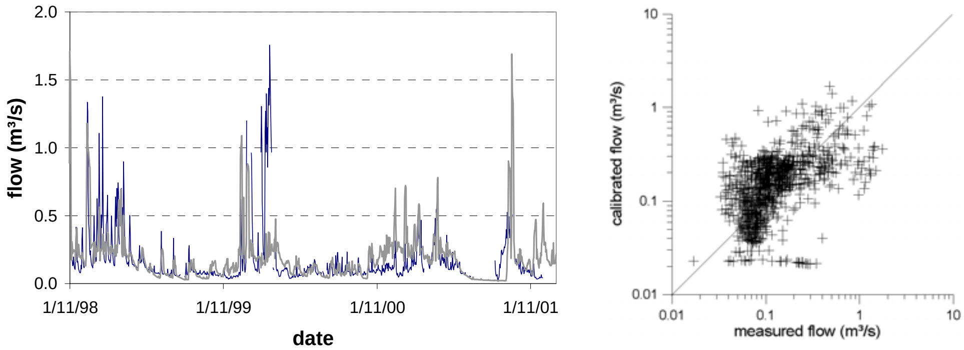


**Figure 4** Comparison of measured ( —— ) and manually calibrated ( —— ) flow data.

An explanation for the low base flow values, can be found in the geological structure of the Nil-catchment. An important part of the groundwater of this catchment is drained to the adjacent river the Train. This is caused by the Brusselian sands, which have a hydraulic conductivity between $10^{-3}$ and $10^{-5}$ m/s and lay above a less permeable socle.

As shown in Figure 4, a good graphical fit was obtained for the measured and manually calibrated flows. Nevertheless, better calibration is possible if seasonally dependent parameters could be adjusted throughout the year. For example, different values for the ESCO parameter during winter and summer, would permit more realistic simulations of water evaporation during both seasons and thereby increase model efficiency.

The results of the auto-calibration are represented in Figure 5. Since a first automated calibration did not give satisfying results for the baseflow, a second automated calibration was performed using a lognormal transformation in order to increase the weights of the baseflow in the OF. In this case, baseflow was well simulated, but peaks due to surface run-off were missed. A square root transformation used in the OF seems to calibrate better peaks originating from surface run-off. As a solution, a multi-objective calibration was performed based on both mentioned transformations.

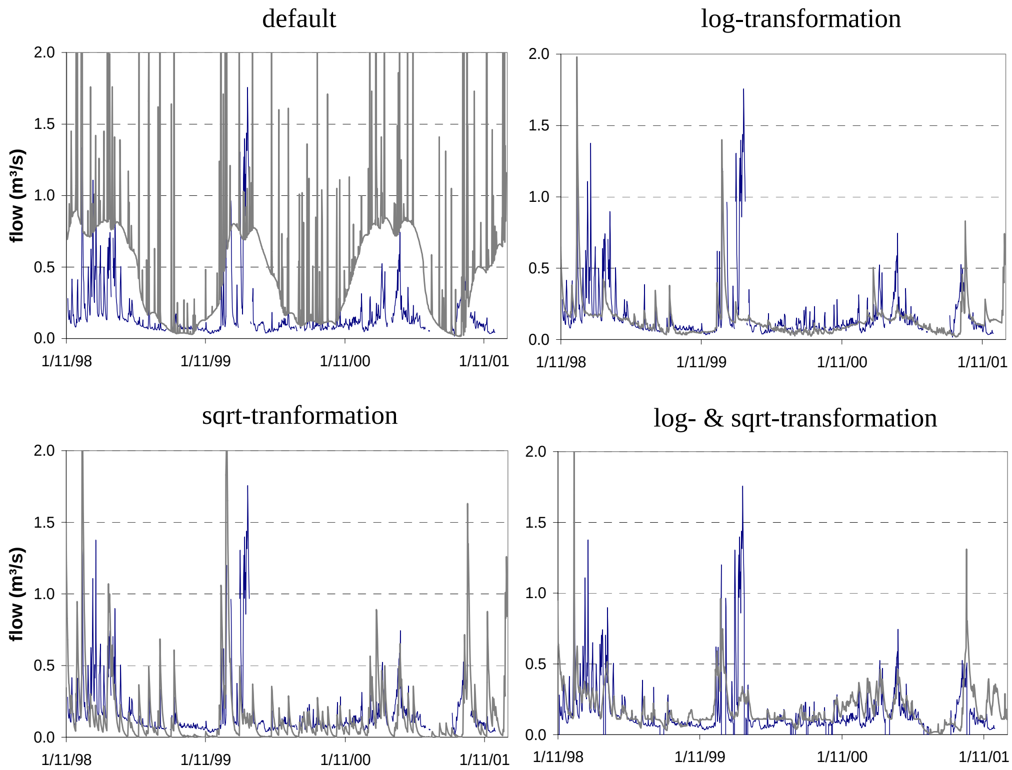


**Figure 5** Comparison of different auto-calibrations of flows: (a) the default values, (b) with a log transformation in the OF, (c) with a square root transformation in the OF and (D) by means of a multi-objective calibration of the two previous OF’s.

For the case of the Nil-catchment, first auto-calibration results seem less satisfying as those achieved by manual calibration. By means of multi-objective calibration, a better fit was achieved. A good mathematical translation of the problem is very important and should further be investigated.

## Conclusions

First, an intensive data collection, the digitisation of soil maps and the calculation of related soil parameters was performed for the Nil catchment. All data was checked upon reliability.

The methodology used to achieve a hydrodynamic model for the Nil-catchment for the purpose of modelling pesticide supply was presented. An LH-OAT sensitivity analysis allowed for the screening of the large set of input parameters. The selected subset of parameters was then used for model calibration. The manual calibration resulted in a good fit for flows. Better results would be possible if seasonally dependent parameters could be adjusted to the season. For the auto-calibration, two transformations in the OF were performed i.e. a logarithmic and a square root. None of them could simulate both baseflow and run-off at the same time. A multi-objective calibration as a combination of both mentioned OF's resulted in a good fit for flows. A good mathematical translation of the problem is very important and should further be investigated.

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