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# Transient water flow in the TOXSWA model (FOCUS versions): concepts and mathematical description

rapporten

P.I. Adriaanse
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WOt Wettelijke Onderzoekstaken Natuur & Milieu

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**Rapport 101**

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**Abstract**
Adriaanse, P.I. & W.H.J. Beltman, 2009. *Transient water flow in the TOXSWA model (FOCUS versions); concepts and mathematical description.* Wageningen, Statutory Research Tasks Unit for Nature and the Environment. WOt-rapport No. 101. 78 p.; 10 Fig.; 2 Tab.; 20 Ref.; 5 Annexes.

The TOXSWA model is used in the pesticide registration procedures in the Netherlands and the EU. This report documents the transient water flow module of TOXSWA, which simulates variable discharges and water depths in the edge-of-field ponds, ditches and streams of the EU FOCUS Surface Water Scenarios at an hourly resolution. It combines water conservation equations with water depth-discharge relations based upon weirs located downstream. In watercourses, backwater curves describe water depths as a function of distance to the weir. The water conservation equations consist of a base flow, excess water fluxes from drainage or runoff and an outflow. The conservation equations have been solved numerically using the finite difference method. A limited verification of the numerical solution has been undertaken. Example runs present model input and output. We recommend implementing a spatially varied flow description with gradually changing water depth in front of the weir.

*Key words*: FOCUS surface water scenarios, pesticide registration, TOXSWA, transient flow

**Referaat**
Adriaanse, P.I. & W.H.J. Beltman, 2009. *Niet-eenparige waterstroming in het model TOXSWA (FOCUS oppervlaktewater scenario's): concepten en wiskundige beschrijving.* Wageningen, Wettelijke Onderzoekstaken Natuur & Milieu, WOt-rapport 101. 78 blz.; 10 fig.; 2 tab.; 20 ref.; 5 bijl.

Het model TOXSWA wordt gebruikt in de toelatingsprocedures van bestrijdingsmiddelen in Nederland en in de EU. Dit rapport documenteert het onderdeel van TOXSWA met een niet-eenparige (dus in de stromingsrichting veranderende) waterstroming. Dit onderdeel simuleert op uurbasis veranderende afvoeren en waterdiepten in de FOCUS Oppervlaktewater Scenario's van de EU: meertjes, sloten en beekjes grenzend aan landbouwpercelen. Waterconserveringsvergelijkingen worden gecombineerd met afvoerformules voor benedenstrooms gelegen stuwen, die het verband tussen de afvoer en de overstorthoogte geven. In de waterlopen beschrijven stuwkrommen het verloop van de waterdiepte met de afstand tot de stuw. De waterconserveringsvergelijkingen bevatten een basisafvoer, overtollige waterfluxen door drainagebuizen of via oppervlakte-afvoer en een uitstroming. De conserveringsvergelijkingen zijn numeriek opgelost met de eindige differentiemethode. De numerieke oplossing is beperkt geverifieerd. Voorbeeldsimulaties tonen de modelinvoer en -uitvoer. We bevelen aan om de wiskundige beschrijving van de waterstroming te verbeteren door een geleidelijk veranderende en discontinue waterstromingsbeschrijving te implementeren, dus met langs de waterloop in- of uitstromend water.

*Trefwoorden:* FOCUS oppervlaktewater scenario's, bestrijdingsmiddelen toelating, TOXSWA, niet-eenparige waterstroming.

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# Contents

# Preface

The first version of the description of the hydrology in TOXSWA for transient flow conditions was written in 1999, when Alterra participated in the EU FOCUS Surface Water Scenarios Working Group (1996-2003). Up to that date, the TOXSWA model had been able to simulate constant flow only, which was judged sufficient for its use in the Dutch registration procedure. In this procedure, exposure to pesticides was calculated in ditches with low, constant flow velocities having received spray drift deposition.

At EU level, it is not only spray drift deposition which is important, but also the entry routes of drainage and surface runoff and erosion. Since drainage and runoff represent considerable water fluxes that enter the watercourse, TOXSWA needed to be able to simulate watercourses with transient flow conditions. Hence, Alterra further developed the hydrological part of the TOXSWA model, which resulted in the FOCUS_TOXSWA model. FOCUS_TOXSWA_1.1.1 was released in May 2003, but its underlying concepts were not fully reported then.

This report fills this gap in the documentation of the transient water flow conditions of the FOCUS_TOXSWA model. Chapter 8 presents some potential further improvements, which may be incorporated in upcoming versions of the TOXSWA model.

The authors wish to thank Jan van Bakel and Erik Querner of the Alterra Centre for Water and Climate for their comments on early drafts of this report, as well as their colleagues Erik van den Berg, Jos Boesten and Mechteld ter Horst of the Environmental Risk Assessment team for their comments over the past years. A special debt of gratitude is owed to Jaap Molenaar of Biometris, who contributed during the final phase of this report.

Finally, this report justifies the existence of Alterra's Software Quality System. The desire to obtain Alterra's Software Quality Level A for FOCUS_TOXSWA stimulated us to finalise the description of the hydrology in the TOXSWA model. This allowed FOCUS_TOXSWA to follow in the footsteps of TOXSWA 1.0, which was the first model meeting the software quality standards formulated by the institute during the 1990s.

*Paulien Adriaanse*
*Wim Beltman*

# Summary

The TOXSWA model simulates pesticide concentrations in edge-of-field watercourses. It was introduced in the Dutch pesticide registration procedure in 1999, where it calculates concentrations in two different ditches with constant discharges and water depths after spray drift deposition. The simulated concentrations are used to assess risks to aquatic ecosystems. The FOCUS surface water scenarios were developed from 1996 to 2003, for use in the EU registration procedure, and the TOXSWA model was selected to simulate exposure in these FOCUS EU scenarios. At EU level, surface runoff and drainage were considered to be important additional pesticide entry routes, next to spray drift deposition. As surface runoff and drainage fluxes result in highly variable water fluxes in watercourses, the TOXSWA model needed to be further developed to be able to simulate variable discharges and water levels. Hence, a transient flow module was developed, which simulates variations in water levels and discharges in edge-of-field watercourses.

Alterra expanded the existing TOXSWA model, version 1.2, which was used in the Dutch registration procedure by developing a transient flow module, describing variable water flow in FOCUS ponds, ditches and streams in a simple, but realistic way.

To do so, we set up water conservation equations for ponds and edge-of-field watercourses, and we defined all incoming and outgoing water fluxes. A small upstream 'catchment', ranging in size from a few hectares to a few hundreds of hectares, delivers its excess water to the watercourse. The runoff fluxes are calculated by the PRZM model, while the drainage fluxes are calculated by the MACRO model. Next, we specified relationships between discharge and water depth. For ponds we used a head-discharge relation for the weir located at the pond outflow. For watercourses with incoming discharges, we calculated the water depth as a function of distance to the weir located downstream: the so-called backwater curves. This resulted in two equations with two unknown variables: the discharge and the water depth. We solved the equations numerically with the aid of the finite-difference method and implemented this transient flow description in the TOXSWA model.

Up to now, the transient flow module has only been parameterised and tested for the layout of the 15 water bodies featuring in the 10 standard FOCUS surface water scenarios. We present example simulations for FOCUS ponds, ditches and streams. In all FOCUS scenarios, a minimum water level of 30 cm is maintained by a weir located downstream. We used hydraulic residence times, i.e. the ratio of water volume and discharge, to characterise the dynamics of flow. In the FOCUS R1 pond, the water depth is virtually constant at 1 m, and the average hydraulic residence time is between 120 and 150 d. The FOCUS D3 ditch has a water depth of 0.30 to 0.31 m; monthly average hydraulic residence times are approximately 0.5 to 5 d. The FOCUS D1 stream has water depths varying between 0.30 and 0.85 m and monthly average hydraulic residence times ranging from a few hours to approximately 1 d. The R2 stream has water depths varying between 0.30 and 1.20 m and monthly average residence times are a few hours only.

We concluded that the convergence of the numerical solution was satisfactory, by comparing concentrations obtained using the usual time and space steps for FOCUS ditches and streams with concentrations obtained using time and space steps that had been reduced by factors of 6 and 5. We recommend operationalising the water balance terms of precipitation, evaporation and seepage in the TOXSWA computer program to obtain more realistic water

level fluctuations, especially in ponds and ditches with low base flows. We suggest that the mathematical description of the transient flow module should be improved by implementing a description for a gradually varying flow in front of a weir, which is also spatially varied, i.e. where water also enters and leaves the flow along its course. Finally, we also recommend repeating the sensitivity and uncertainty analysis for this new version of the TOXSWA model and testing the transient flow module against field measurements in ponds or small watercourses located at the downstream end of small catchments.

# Samenvatting

Het model TOXSWA wordt gebruikt om concentraties bestrijdingsmiddelen in aan landbouwpercelen grenzende waterlopen te simuleren. Het model werd in 1999 ingevoerd in de Nederlandse toelatingsprocedure voor bestrijdingsmiddelen om concentraties te berekenen in twee verschillende sloten met constante afvoer en waterdiepte ten gevolge van drift bij gewasbescherming. De gesimuleerde concentraties worden gebruikt bij het schatten van het risico voor aquatische ecosystemen. De FOCUS Oppervlaktewater Scenario's zijn ontwikkeld in de periode 1996 tot 2003 om bij de toelatingsprocedure van de EU te gebruiken. Het model TOXSWA werd gekozen voor het simuleren van de blootstelling in deze FOCUS-scenario's. Op EU-niveau werden oppervlakte-afvoer en drainage beschouwd als belangrijke routes waarlangs bestrijdingsmiddelen in waterlopen terecht kunnen komen, naast drift bij gewasbescherming. Aangezien waterfluxen door oppervlakte-afvoer en drainage leiden tot sterk variërende afvoer in de waterlopen, betekende dit dat het model TOXSWA verder moest worden ontwikkeld zodat er ook variabele afvoeren en waterdiepten mee konden worden gesimuleerd. Hiervoor werd een module voor niet-eenparige (dus in de stromingsrichting veranderende) waterstroming ontwikkeld, waarmee variaties in waterdiepte kunnen worden gesimuleerd in waterlopen naast landbouwpercelen.

Alterra heeft het bestaande model TOXSWA (versie 1.2), dat gebruikt werd in de Nederlandse toelatingsprocedure, uitgebreid met een module voor niet-eenparige waterstroming, die de variabele waterstroming in de meertjes, sloten en beken uit de FOCUS-scenario's op een eenvoudige maar realistische manier kan simuleren.

Hiertoe werden waterconserveringsvergelijkingen opgesteld voor meertjes en waterlopen naast landbouwpercelen, en zijn alle inkomende en uitgaande waterfluxen gedefinieerd. Er is uitgegaan van een klein stroomopwaarts gelegen 'stroomgebied', in grootte variërend van enkele hectaren tot enkele honderden hectaren, van waaruit overtollig water wordt afgevoerd naar de waterloop. De waterfluxen door oppervlakte-afvoer worden berekend met behulp van het model PRZM, terwijl de fluxen door drainage worden berekend met behulp van het model MACRO. Vervolgens zijn de verbanden gespecificeerd tussen afvoer en waterdiepte. Voor meertjes werd een afvoerkromme gebruikt die de relatie tussen afvoer en overstorthoogte geeft voor een stuw bij het uitstroompunt van het meertje. Voor waterlopen met instromend water hebben we het verloop van de waterdiepte met de afstand tot de benedenstrooms gelegen stuw berekend als zogenaamde stuwkrommen. Dit resulteerde in twee vergelijkingen met twee onbekenden: de afvoer en de waterdiepte. Deze vergelijkingen zijn numeriek opgelost met de eindige differentie-methode, waarna deze beschrijving van de niet-eenparige stroming werd ingebracht in het model TOXSWA.

Tot dusverre zijn de parameterisatie en het testen van de module voor niet-eenparige stroming beperkt gebleven tot de 15 waterlichamen die worden gedefinieerd in de 10 standaard FOCUS-scenario's voor oppervlaktewater. In het rapport zijn voorbeeldsimulaties opgenomen voor de in FOCUS gedefinieerde meertjes, sloten en beken. In alle FOCUS-scenario's wordt een minimale waterdiepte van 30 cm in stand gehouden door een benedenstrooms gelegen stuw. De hydraulische verblijftijd, dit wil zeggen de verhouding tussen het watervolume en de afvoer, werd gebruikt om de stromingsdynamiek te karakteriseren. In het meertje type R1 in FOCUS is de waterdiepte vrijwel constant 1 m, en de gemiddelde hydraulische verblijftijd ligt tussen de 120 en 150 dagen. Bij de sloot D3 varieert de waterdiepte tussen 0,30 en 0,31 m, terwijl het maandgemiddelde van de verblijftijd varieert van 0,5 tot 5 dagen. In de beek D1

varieert de waterdiepte tussen 0,30 en 0,85 m, terwijl het maandgemiddelde van de verblijftijd uiteenloopt van enkele uren tot ca. 1 dag. De beek R2 heeft een waterdiepte die varieert tussen 0,30 en 1.20 m, met een maandgemiddelde voor de verblijftijd van slechts enkele uren.

Door de concentraties die werden verkregen met de voor de FOCUS-waterlopen gebruikelijke tijd- en plaatsstappen te vergelijken met de concentraties die werden verkregen met 5 en 6 maal zo kleine tijd- en plaatsstappen, kon worden vastgesteld dat de convergentie van de numerieke oplossing adequaat is. Wij bevelen aan om de waterbalanstermen neerslag, verdamping en kwel in TOXSWA te operationaliseren om meer realistische waterdiepte-fluctuaties te verkrijgen, met name in meertjes en sloten met een geringe basisafvoer. Voorts bevelen wij aan om de wiskundige beschrijving van de module voor niet-eenparige water-stroming te verbeteren door het implementeren van een beschrijving van een geleidelijk veranderende waterstroming vóór de stuw, die tevens discontinu is, dus met langs de waterloop in- of uitstromend water. Ten slotte adviseren wij om een nieuwe gevoeligheids- en onzekerheidsanalyse uit te voeren voor deze nieuwe versie van TOXSWA, en om de module voor niet-eenparige waterstroming te ijken met behulp van veldmetingen in meertjes of kleine waterlopen aan de benedenstroomse zijde van een klein stroomgebied.

# 1 Introduction

The TOXSWA model (TOXic substances in Surface WAter) describes pesticide behaviour in a watercourse, including its sediment. It is a pseudo-two-dimensional model, which calculates pesticide concentrations in the water layer in a horizontal direction only, and concentrations in the sediment layer in both horizontal and vertical directions. TOXSWA considers four processes: (i) transport, (ii) transformation, (iii) sorption and (iv) volatilisation (Adriaanse, 1996; Adriaanse, 1997). TOXSWA 1.0 was released on 23 April 1996 (Beltman *et al*, 1996).

The TOXSWA 1.2 model has been applied in the Dutch pesticide registration procedure since 1 June 1999. The Board for the Authorisation of Plant Protection Products and Biocides (Ctgb) uses TOXSWA 1.2 to simulate exposure concentrations in two different edge-of-field ditches with constant, low flow to assess risks of pesticides to the aquatic ecosystem (Beltman and Adriaanse, 1999a and 1999b).

This report describes the hydrology of the FOCUS_TOXSWA model[1]. FOCUS_TOXSWA is used to simulate the behaviour of pesticides in the FOCUS Surface Water Scenarios, consisting of ponds, ditches and streams. (FOCUS, 2001; http://focus.jrc.ec.europa.eu/sw/). Exposure assessment in these scenarios is an obligatory part of the EU registration procedure under EU Directive 91/414/EEC.

The FOCUS scenarios display transient flow conditions. Discharges and water depths vary in time in the FOCUS ponds, ditches and streams, because drainage and runoff are important entry routes for pesticides. The transient flow hydrology in the TOXSWA model was developed within the context of the FOCUS Surface Water Scenarios Working Group and has only been tested for the lay-out of the FOCUS scenarios.

Summarising, TOXSWA version 1.2 describes pesticide behaviour in watercourses with constant water flow, while FOCUS_TOXSWA versions describe pesticide behaviour in water bodies with transient flow conditions. Both models also describe pesticide behaviour in stagnant, ideally mixed reservoirs, such as ponds or laboratory water-sediment systems.

This report is complementary to Adriaanse (1996), which means that the content of Adriaanse (1996) applies not only to TOXSWA version 1.2 but also to the FOCUS_TOXSWA model.

Chapter 2 presents water conservation equations for ponds and for watercourses receiving excess water from surrounding areas. These equations include two unknown variables, the water depth and the discharge. A method to calculate the water depth as a function of discharge in ponds and watercourses is described in Chapter 3. Chapter 4 describes the upper and lower boundary conditions of the conservation equation, as well as the initial condition. Lower boundaries are formed by weirs maintaining the water level. In Chapter 5, the water conservation equations are solved numerically, and a limited verification of the numerical solution is described in Chapter 6. Chapter 7 presents some example runs for FOCUS ponds, ditches and streams. Chapter 8 formulates conclusions and recommendations.

[1] Two versions of FOCUS_TOXSWA have been released up to now: FOCUS_TOXSWA_1.1.1 (released 13 May 2003) and FOCUS_TOXSWA_2.2.1 (released 21 December 2005, Beltman *et al*, 2006).

In each chapter, we illustrate how the concepts have been applied in the FOCUS Surface Water Scenarios (FOCUS, 2001). The FOCUS Scenarios cover a realistic range of surface water bodies, topography, climate, soil type and agricultural management practices in the major agricultural areas of the European Union. They take into account all relevant pesticide entry routes, based on Good Agricultural Practice: spray drift deposition, drainage and surface runoff and erosion. For reasons of simplicity, the FOCUS Working Group assumed that the entry routes of drainage and surface runoff/erosion are mutually exclusive, which is why the FOCUS Surface Water Scenarios are subdivided into so-called Drainage scenarios (D1 – D6) in which pesticides enter the water body via spray drift deposition and drainage, and Runoff scenarios (R1 - R4) with spray drift deposition and runoff/erosion as entry routes. The D scenarios may be associated with ponds, ditches and streams, while the R scenarios are only associated with ponds or streams.

# 2 Water conservation equations

## 2.1 Introduction

This chapter presents the water conservation equations for ponds and watercourses. It also discusses how these water bodies and their water fluxes have been defined in more detail for the FOCUS Surface Water Scenarios.

## 2.2 Ponds

A pond is a rectangular reservoir with vertical sides having an incoming and an outgoing water flow. Fields that may be located at its left-hand and right-hand banks deliver their excess water into the pond; these fields are called the contributing area (Figure 1). The total incoming flow consists of a constant[2] base flow plus the excess water from the contributing area, delivered into the pond. The pond outflow occurs across a weir. The incoming excess water from the contributing area originates from e.g. drain pipes or surface runoff. Since it is a function of precipitation, soil type, land use, slope etc., the excess water fluxes vary in time.

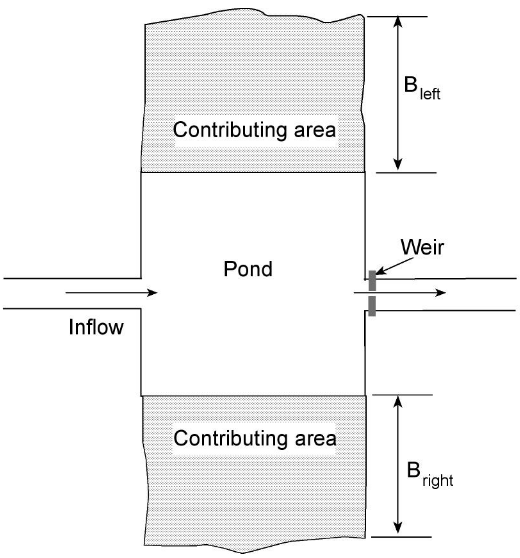


*Figure 1 Schematic layout of the pond in the TOXSWA model with inflow, contributing area with total width $B_{left}$+$B_{right}$ and weir*

[2] In this report, 'constant' always refers to constant in time, and the term 'uniform' is used to refer to uniform flow conditions as used in hydraulics, where it means constant in space.

A water conservation equation can be set up for an elemental volume $\Delta x\ b_{pond}$ of the pond (Figure 2).

At time *t:*

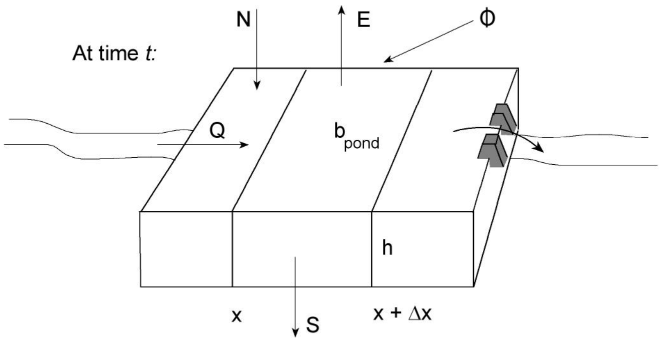


*Figure 2. Elemental volume in the pond at time t with its main water balance components. At time t+Δt, the water depth h has become h+Δh*

Here,

| | | |
|---|---|---|
| $x$ | = | distance in the direction of flow in the pond (L)( space)[3] |
| $Q_{pond,x}$ | = | discharge, i.e. volume flux of water passing through a vertical cross-section of the pond at distance $x$ ($L^3.T^{-1}$) (time, space) |
| $h_{pond}$ | = | water depth (L) (time) |
| $b_{pond}$ | = | bottom width of the pond (L) |
| $\Phi_{pond}$ | = | lineic volume flux, that is the volume of water entering the pond from drain pipes or runoff from the contributing area, divided by pond length and by time ($L^3.\ L^{-1}.T^{-1}$) (time) |
| $N_{pond}$ | = | areic[4] volume flux from precipitation, i.e. volume of precipitation divided by the pond surface area and by time; the flux is positive in a downward direction ($L^3.L^{-2}.T^{-1}$) (time) |
| $E_{pond}$ | = | areic volume flux from evaporation, i.e. volume of water evaporated divided by the pond surface area and by time; the flux is negative in an upward direction ($L^3.L^{-2}.T^{-1}$) (time) |
| $S_{pond}$ | = | areic volume flux from seepage, i.e. volume of water seeping upward or downward, divided by the appropriate sediment surface area and by time; the flux is positive in a downward direction ($L^3.L^{-2}.T^{-1}$) (time) |

The water conservation equation for an elemental pond volume $h\Delta x b_{pond}$ reads:

Increase in water volume = inflow – outflow + excess water from contributing area + rainfall – evaporation – seepage[5]

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[3] The dimensions of the symbols introduced are given between the first pair of brackets. L stands for length, T for time, M for mass (Schurer and Rigg, 1980). The quantities on which the introduced variable depends are given between the second pair of brackets.

[4] Areic means that it is divided by the area concerned.

[5] The water balance terms of precipitation, evaporation and seepage have not been operationalized for ponds in FOCUS_TOXSWA versions 1.1.1 and 2.2.1.

Written in terms of differentials:

$$\left(\Delta x b_{pond}\right)h_{t+\Delta t} - \left(\Delta x b_{pond}\right)h_t =$$
$$\Delta t\left(Q_{pond,x} - Q_{pond,x+\Delta x} + \Phi_{pond}\Delta x + N_{pond}\Delta x b_{pond} + E_{pond}\Delta x b_{pond} - S_{pond}\Delta x P_{z=0}\right) \Leftrightarrow$$
$$\left(\Delta x b_{pond}\right)\Delta h = \Delta t\left(-\Delta Q_{pond,x} + \Phi_{pond}\Delta x + N_{pond}\Delta x b_{pond} + E_{pond}\Delta x b_{pond} - S_{pond}\Delta x P_{z=0}\right) \Leftrightarrow$$
$$\frac{\Delta h}{\Delta t} = -\frac{\Delta Q_{pond,x}}{\Delta x\, b_{pond}} + \frac{\Phi_{pond}}{b_{pond}} + N_{pond} + E_{pond} - S_{pond}\frac{P_{z=0}}{b_{pond}}$$

with
- $t$ = time (T)
- $P_{z=0}$ = length of wetted perimeter at depth $z$ = 0, via which exchange between water and sediment occurs (for more details, see section 3.2 of Adriaanse, 1996) (L)

Taking the limit for Δt approaching zero we obtain the following differential equation:

$$\frac{\partial h}{\partial t} = -\frac{\partial Q_{pond,x}}{\partial x\, b_{pond}} + \frac{\Phi_{pond}}{b_{pond}} + N_{pond} + E_{pond} - S_{pond}\frac{P_{z=0}}{b_{pond}} \qquad \textit{eq. 1}$$

The lineic volume flux from the contributing area equals:

$$\Phi_{pond} = B_{contr.area}\, q_{rodr,pond} \qquad \textit{eq. 2}$$

and

$$B_{contr.area} = B_{left} + B_{right} \qquad \textit{eq. 3}$$

with
- $B_{left}$ = width (perpendicular to the pond length) of the fields located at the left-hand bank of the pond, discharging their excess water into the pond (L)
- $B_{right}$ = width (perpendicular to the pond length) of the fields located at the right-hand bank of the pond, discharging their excess water into the pond (L)
- $B_{contr.area}$ = total width (perpendicular to the pond length) of the fields, the so-called contributing area, discharging its excess water into the pond (L)
- $q_{rodr,pond}$ = areic volume flux of excess water of the contributing area, that is, the volume of excess water from e.g. pipe drainage or surface runoff into the pond, divided by the excess water-generating surface area and by time ($L^3.L^{-2}.T^{-1}$) (time)

The (upward or downward) seepage in the sediment equals:

$$S_{pond} = \frac{B_{contr.area}}{P_{z=0}}\, q_{sub,pond} \qquad \textit{eq. 4}$$

with
- $q_{sub,pond}$ = areic volume flux from subsurface flow, that is, the volume of water drained or supplied via subsurface flow, based upon the surface area of the contributing area. The flux is negative for upward flow in the perimeter of exchange $P_{z=0}$ (i.e.

drainage from the contributing area) and positive for infiltration into the perimeter of exchange $P_{z=0}$ (i.e. water supplied to the contributing area). ($L^3.L^{-2}.T^{-1}$) (time)

We considered the pond to be an ideally mixed reservoir with a uniform water depth *h*. The terms $\Phi_{pond}$, *N, E* and *S* are not a function of distance in the pond, which means that all terms in the water conservation equation can be simply integrated over *x*, from one end of the pond to the other, $x = 0$ and $x = l_{pond}$. This results in:

$$\frac{dhl_{pond}}{dt} = -\left( \frac{Q_{pond,l_{pond}} - Q_{pond,0}}{b_{pond}} \right) + \frac{\Phi_{pond}}{b_{pond}} l_{pond} + \left( N + E - S \frac{P_{z=0}}{b_{pond}} \right) l_{pond} \Leftrightarrow$$

$$\frac{dhl_{pond} b_{pond}}{dt} = \left( Q_{pond,o} - Q_{pond,l_{pond}} \right) + \Phi_{pond} l_{pond} + \left( N + E - S \frac{P_{z=0}}{b_{pond}} \right) l_{pond} b_{pond} \Leftrightarrow \quad \textit{eq. 5}$$

$$\frac{dV_{pond}}{dt} = \left( Q_{pond,o} - Q_{pond,l_{pond}} \right) + \Phi_{pond} l_{pond} + (N + E) l_{pond} b_{pond} - S P_{z=o} l_{pond}$$

and

$$V_{pond} = hb_{pond} l_{pond} \qquad \textit{eq. 6}$$

with

$l_{pond}$ = length of the pond in the direction of flow (L)
$V_{pond}$ = volume of water in the pond ($L^3$) (time)

The water volume $V_{pond}$ depends on the water depth *h(t)*. In section 3.2 we determine the water depth as a function of time, at the weir located at the outflow of the pond.

## 2.3 Ponds in the FOCUS Surface Water Scenarios

The ponds in the FOCUS Surface Water Scenarios are square and measure 30 by 30 m, with a weir located at the pond outflow. The base flow is constant and the three FOCUS ponds have base flows of 3.19 (D4 scenario), 2.23 (D5 scenario) and 5.75 (R1 scenario) $m^3/d$. The excess water fluxes from the contributing area are often zero, with a maximum of 0.77 mm/h for ponds receiving drainage fluxes (D5 scenario) and a maximum of 1.39 mm/h for ponds receiving runoff fluxes (R1, weather year used for pesticide applications from March to May, i.e. spring applications). The contributing area (i.e. $l_{pond}$ $B_{pond}$) measures 4500 $m^2$, corresponding to a land:water ratio of 5.

The excess water from pipe-drained contributing areas consists of the water fluxes leaving the drain pipes. This is simulated by the MACRO model (Jarvis, 1994; Jarvis, 2001; FOCUS, 2001; http://focus.jrc.ec.europa.eu/sw/). The variable $q_{rodr,pond}$ therefore equals:

$$q_{rodr,pond} = q_{dr,MACRO} \qquad \textit{eq. 7}$$

with

$q_{dr,MACRO}$ = areic volume flux of pipe drainage water from the contributing area as calculated by MACRO ($L^3.L^{-2}.T^{-1}$) (time)

The excess water from contributing areas with runoff consists of surface runoff plus a smaller subsurface drain flow. The surface runoff flow may contain pesticide mass, while the smaller, less dynamic subsurface drain flow does not contain pesticides and part of it is assumed to enter the water layer directly (which was done because the term S is not operational in the FOCUS_ TOXSWA model). This is simulated by the PRZM model (Carsel *et al*, 1995; FOCUS, 2001; http://focus.jrc.ec.europa.eu/sw/). For the FOCUS Runoff scenarios, the variable $q_{rodr,pond}$ thus combines the surface runoff and part of the subsurface drain flow:

$$q_{rodr,pond} = q_{ro,PRZM} + F_{per,pond}\, q_{down,PRZM} \qquad \textit{eq. 8}$$

with

$q_{ro,PRZM}$ = areic volume flux of surface runoff water from the contributing area, as calculated by PRZM ($L^3.L^{-2}.T^{-1}$) (time)

$q_{down,PRZM}$ = downward areic volume flux of water at 1 m soil depth in the contributing area, as calculated by PRZM ($L^3.L^{-2}.T^{-1}$) (time)

$F_{per,pond}$ = fraction of downward areic volume flux of water at 1 m soil depth in the contributing area that flows into the pond (1)

## 2.4 Watercourses

The TOXSWA model calculates pesticide behaviour in watercourses at the edge-of-field scale, i.e. watercourses with a maximum length of a few hundred metres adjacent to a single field. The hydrological submodel of TOXSWA therefore focuses on the same scale, i.e. that of a single edge-of-field watercourse.

The TOXSWA watercourse[6] is located at the downstream end of a small catchment, enabling it to simulate a realistic transient flow regime. The size of the catchment may vary from a few to a few hundred hectares. A small weir located downstream maintains the water level next to the adjacent field at a preferred minimum depth (Figure 3). The requirement that the edge-of-field watercourse should have a minimum depth matches the current aquatic risk assessment procedures for pesticide registration, which do not consider temporary water bodies.

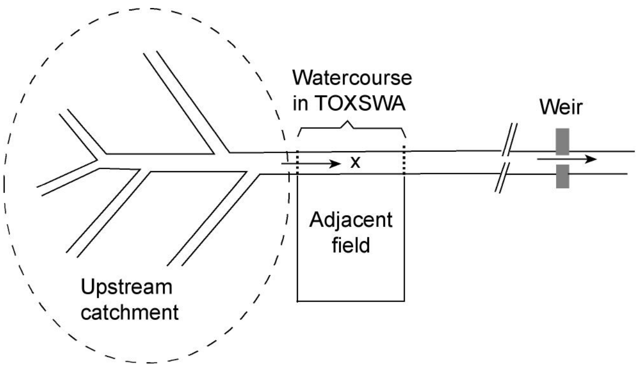



*Figure 3. Schematic layout of the watercourse of the TOXSWA model with adjacent field, upstream catchment and weir*

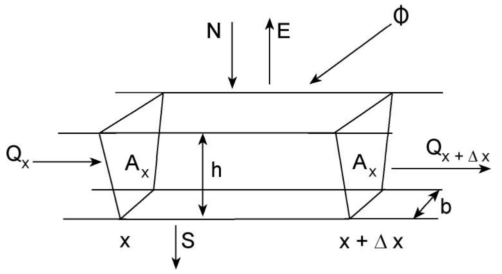
[6] In this report, the term 'edge-of-field watercourse' specifically refers to the relatively short reach of the watercourse immediately adjacent to the field receiving pesticide applications, for which the water (and pesticide mass) conservation equations are set up. The term 'watercourse' may also refer to the entire watercourse, e.g. including the reach up to the weir.

The edge-of-field watercourse has a trapezium-shaped cross-section. The inflow across the upper boundary varies in time and consists of two components: (i) a small base flow, which may be constant and (ii) a variable excess water flow from the catchment.

In addition to the inflow of water across the upper boundary, there is a lateral inflow, consisting of the excess water from the adjacent field. The excess water originates from e.g. drain pipes or surface runoff from the adjacent field. It is a function of precipitation, soil type, land use, slope etc.

We simplified the water flow in the edge-of-field watercourse by assuming that the water depth is constant over the length of this watercourse, so the water depth only varies in time. Because excess water from the adjacent field enters the watercourse, the flux of water is a function of the distance in the direction of flow. A one-dimensional water conservation equation can be developed for the elemental volume $A\Delta x$, in which $A$ represents the cross-sectional surface area perpendicular to the direction of flow.

At time *t*:




At time *t+ Δt*:

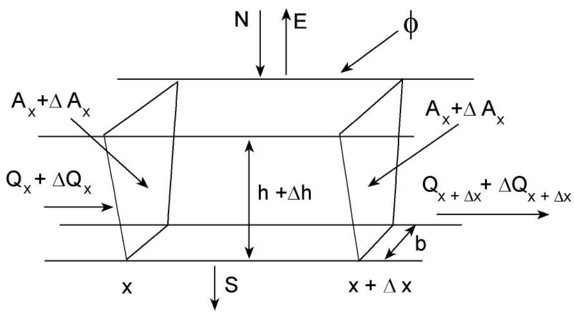



*Figure 4. Elemental volume in the edge-of-field watercourse at times t and t+Δt, with its main water balance components*

Here

| | | |
|---|---|---|
| $x$ | = | distance in the direction of flow (L) (space) |
| $Q_x$ | = | discharge, i.e. volume flux of water passing through a vertical cross-section of the watercourse at location $x$ ($L^3.T^{-1}$) (time, space). |
| $A$ | = | cross-sectional area of flow ($L^2$) (time) |
| $h$ | = | water depth (L) (time) |
| $b$ | = | bottom width of the watercourse (L) |
| $\Phi$ | = | lineic volume flux from drainage or runoff, that is, the volume of water entering the watercourse from drain pipes or runoff from an adjacent field, divided by watercourse length and by time ($L^3.L^{-1}. T^{-1}$) (time) |

| | | |
|---|---|---|
| $N$ | = | areic volume flux from precipitation, i.e. volume of precipitation divided by an appropriate watercourse surface area and by time; the flux is positive in a downward direction ($L^3.L^{-2}.T^{-1}$) (time) |
| $E$ | = | areic volume flux from evaporation, i.e. volume of water evaporated, divided by the appropriate watercourse surface area and by time; the flux is negative in an upward direction ($L^3.L^{-2}.T^{-1}$) (time) |
| $S$ | = | areic volume flux from seepage, i.e. volume of water seeping upward or downward, divided by the appropriate sediment surface area and by time; the flux is positive in a downward direction ($L^3.L^{-2}.T^{-1}$) (time) |

The water conservation equation reads:

increase in water volume = inflow – outflow + incoming lateral flow + rainfall – evaporation – seepage[7]

Written in terms of differentials:

$$A_{t+\Delta t}\Delta x - A_t\Delta x = \Delta t\left(Q_x - Q_{x+\Delta x} + \cdot\Phi\Delta x + N\Delta xO + E\Delta x \cdot O - S\Delta xP_{z=0}\right) \Leftrightarrow$$
$$\Delta A_t\,\Delta x = \Delta t\left(-\Delta Q_x + \Phi\Delta x + N\Delta xO + E\Delta xO - S\Delta xP_{z=0}\right)$$

Hence,

$$\frac{\Delta A_t}{\Delta t} = -\frac{\Delta Q_x}{\Delta x} + \Phi + NO + EO - SP_{z=0}$$

with

| | | |
|---|---|---|
| $t$ | = | time (T) |
| $O$ | = | width of water surface (L) (time) |
| $P_{z=0}$ | = | length of wetted perimeter at depth $z$ = 0, via which exchange between water and sediment occurs (for more details, see section 3.2 of Adriaanse, 1996) (L) |

Taking the limit for $\Delta t$ and $\Delta x$ approaching zero, we obtain the following differential equation:

$$\frac{\partial A}{\partial t} = -\frac{\partial Q_x}{\partial x} + \Phi + NO + EO - SP_{z=0} \qquad \textit{eq. 9}$$

This is the water conservation equation for the water layer in the edge-of-field watercourse. Mark that it is nearly identical to the one for the pond (eq.1), the only difference being the shape of the wetted cross-section of the water body.

7 The water balance terms of precipitation, evaporation and seepage have not been operationalized for watercourses in FOCUS_TOXSWA.

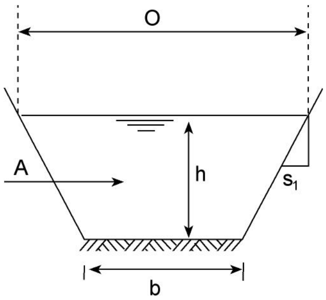


*Figure 5. Cross-section of the watercourse*

The equation for the cross-sectional area of the flow reads (Figure 5):

$$A = bh + h^2 s_1 \qquad \textit{eq. 10}$$

With
$s_1$ = side slope (horizontal/vertical) (1)

The width of the water surface O equals (Figure 5):

$$O = b + 2hs_1 \qquad \textit{eq. 11}$$

The lineic volume flux from the adjacent field equals:

$$\Phi = Bq_{rodr} \qquad \textit{eq. 12}$$

with
B = width of the adjacent field (perpendicular to the watercourse) discharging its excess water into the watercourse (L)
$q_{rodr}$ = areic volume flux of excess water from the adjacent field, that is, the volume of excess water from e.g. pipe drainage or surface runoff into the watercourse, divided by the surface area of the excess water-generating adjacent field and by time (L3.L-2.T-1) (time)

The (upward or downward) seepage in the sediment equals:

$$S = \frac{B}{P_{z=0}} q_{sub} \qquad \textit{eq. 13}$$

with
$q_{sub}$ = areic volume flux from subsurface flow, i.e. volume of water drained or supplied via subsurface flow, based on the surface area of the adjacent field. The flux is negative for upward flow in the sediment (i.e. drainage from the adjacent field) and positive for infiltration into the sediment (i.e. water supplied to the adjacent field). ($L^3.L^{-2}.T^{-1}$) (time)

## 2.5 Watercourses in the FOCUS Surface Water Scenarios

The FOCUS Surface Water Scenarios include two types of watercourses: ditches and streams. Both ditches and streams are 100 m long. Ditches have small (2 ha) upstream catchments, while stream catchments have a size of 100 ha. The adjacent field is rectangular and measures 1 ha (i.e. extending for 100 m along the watercourse). The base flow is constant and ranges from 0.012 (D2) to 3.7 (D6) $m^3/d$ for FOCUS ditches and from 0.60 (D2) to 280 (R2) $m^3/d$ for FOCUS streams. The excess water fluxes for the adjacent field are often zero.

The maximum values of the excess water fluxes are listed in Table 1 (drainage fluxes) and Table 2 (runoff fluxes). The excess water fluxes from the adjacent field are also used for the excess water fluxes originating from the upstream catchments, so the hydrologic behaviour of the adjacent field was assumed to also represent the hydrologic behaviour of the upstream catchment.

*Table 1. Maximum drainage fluxes in mm/h and mm/d for the FOCUS D scenarios. The numbers refer to the winter cereals crop. The year indicates the weather year used. The simulation period for D scenarios is 16 months, so the weather year, e.g. 1985, indicates that the model run covered the period from 1 January 1985 to 30 April of the next year, i.e. 1986.*

| Scenario | Weather year | Maximum drainage flux | |
|---|---|---|---|
| | | mm/h | mm/d |
| D1 | 1982 | 0.47 | 8.96 |
| D2 | 1986 | 1.40 | 11.71 |
| D3 | 1992 | 0.09 | 2.19 |
| D4 | 1985 | 0.30 | 5.48 |
| D5 | 1978 | 0.77 | 10.93 |
| D6 | 1986 | 1.70 | 21.58 |

*Table 2. Maximum runoff fluxes in mm/h and mm/d for the FOCUS R scenarios. The numbers refer to the maize crop. The weather year is selected according to the pesticide application period (applications in March-May are called spring applns, applications in June-September summer applns and applications in October to February autumn applns), and the year mentioned indicates the start of the 12-month simulation period. E.g. the R2 summer applications weather year starts 1 June 1989 and ends 31 May 1990.*

| Application period/scenarios | Weather year | Maximum runoff flux | |
|---|---|---|---|
| | | mm/h | mm/d |
| Spring applns | | | |
| R1 | 1984 | 1.39 | 10.28 |
| R2 | 1977 | 1.22 | 29.17 |
| R3 | 1980 | 1.17 | 24.55 |
| R4 | 1984 | 1.74 | 41.79 |
| | | | |
| Summer applns | | | |
| R1 | 1978 | 1.35 | 13.87 |
| R2 | 1989 | 1.27 | 30.56 |
| R3 | 1975 | 1.21 | 29.03 |
| R4 | 1985 | 1.86 | 29.71 |
| | | | |
| Autumn applns | | | |
| R1 | 1978 | 1.35 | 13.87 |
| R2 | 1977 | 1.22 | 29.17 |
| R3 | 1980 | 1.17 | 24.55 |
| R4 | 1979 | 1.63 | 39.03 |

The excess water from pipe-drained fields consists of the water fluxes leaving the drain pipes. This is simulated by the MACRO model (Jarvis, 1994; Jarvis, 2001; FOCUS, 2001; http://focus.jrc.ec.europa.eu/sw). Hence, the variable $q_{rodr}$ equals:

$$q_{rodr} = q_{dr,MACRO} \qquad \textit{eq. 14}$$

with

$q_{dr,MACRO}$ = areic volume flux of pipe drainage water from the adjacent field as calculated by MACRO ($L^3.L^{-2}.T^{-1}$) (time)

The excess water from fields with runoff consists of surface runoff plus a smaller subsurface drain flow. The surface runoff flow may contain pesticide mass. The smaller, less dynamic subsurface drain flow does not contain pesticides, and part of it is assumed to enter the water layer directly (which was done because the term S is not operational in the FOCUS_TOXSWA model). This is simulated by the PRZM model (Carsel *et al*, 1995; FOCUS, 2001; http://focus.jrc.ec.europa.eu/sw/). For the FOCUS Runoff scenarios, the variable $q_{rodr}$ thus combines the surface runoff and part of the subsurface drain flow:

$$q_{rodr} = q_{ro,PRZM} + F_{per} q_{down,PRZM} \qquad \textit{eq. 15}$$

with

$q_{ro,PRZM}$ = areic volume flux of surface runoff water from the adjacent field as calculated by PRZM ($L^3.L^{-2}.T^{-1}$) (time)

$q_{down,PRZM}$ = downward areic volume flux of water at 1 m soil depth in the adjacent field as calculated by PRZM ($L^3.L^{-2}.T^{-1}$) (time)

$F_{per}$ = fraction of downward areic volume flux of water at 1 m soil depth in the adjacent field that flows into the watercourse (1)

# 3 Relations between discharge and water depth

## 3.1 Introduction

The water conservation equations of the previous chapter include two unknown variables: the discharge $Q$, and the water depth $h$ (or cross-sectional area of flow $A$, which is determined by $h$). Solving the conservation equations requires a second relationship, relating discharge and water depth. Such a relationship is presented below for ponds as well as for watercourses.

## 3.2 Ponds, including FOCUS ponds

A weir, located at the outlet of the pond, governs the pond's discharge. A so-called 'head-discharge relationship' defines the discharge as a function of the water level above the crest of a weir. For broad-crested weirs which are freely discharging, such head-discharge relationships read (Working Group on Small Hydraulic Structures, 1978):

$$Q_{weir,pond} = C_{pond}\, w_{crest,pond}\, h_{crest,pond}^{\frac{3}{2}} \qquad \textit{eq. 16}$$

with

$Q_{weir,pond}$ = discharge across the weir ($L^3.T^{-1}$) (time)
$C_{pond}$ = discharge coefficient, depending on weir characteristics ($L^{½}\ T^{-1}$)
$w_{crest,pond}$ = width of the crest of the weir (L)
$h_{crest,pond}$ = upstream water level over the weir crest, also called head (L)

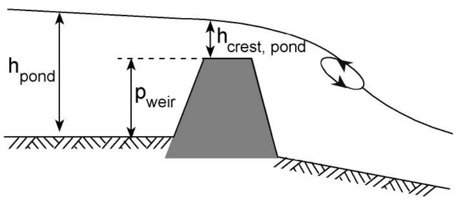



*Figure 6. Water depth in the pond*

The water depth in the pond is (Figure 6):

$$h_{pond} = p_{weir} + h_{crest,pond} \qquad \textit{eq. 17}$$

with

$p_{weir}$ = height of the weir crest above the pond bottom (L)

In the FOCUS Surface Water Scenarios, the weir in the pond has its crest at 1.0 m above the pond bottom and the crest is 0.50 m wide. The discharge coefficient of the weir equals 1.7 $m^{½}.s^{-1}$ (Ministère des Relations Extérieures, Coopération et Développement, 1984). The head over the weir crest does not exceed a few centimetres, as incoming base flows and excess water fluxes from the contributing areas are small compared to the pond volume.

## 3.3 Watercourses, including the FOCUS ditches and streams

The edge-of-field watercourse is fed by excess water emerging from the upstream catchment as well as by lateral excess water fluxes originating from the adjacent field; the size of the excess water fluxes varies in time. The discharge of the watercourse is therefore a function of both time and distance. In hydraulic terms: the flow in the watercourse is both *unsteady* (i.e. varies in time) and *spatially varied or discontinuous* (water entering or leaving along the course of flow). This is a complex form of flow to describe in a hydraulically correct manner (Chow, 1959).

To obtain a simplified relationship between $Q$ and $h$, we defined another watercourse. We called this watercourse the auxiliary channel, to avoid confusion with the original edge-of-field watercourse and because later on, we used it as an auxiliary tool to solve the water conservation equation. In our auxiliary channel we simplified the complex unsteady, discontinuous flow into a sequence of steady and continuous flows, that is, a sequence of steady state situations with continuous flow.

The edge-of-field watercourse has a weir located somewhere in the downstream direction, which influences the water level in the watercourse. As one moves in the downstream direction to the weir, the depth of flow changes gradually, which is why this type of flow is called *gradually varied flow*. We maintained this gradually varied flow type in the auxiliary channel. Unlike the situation here, section 2.4 simplified the water flow by assuming that the water depth in the edge-of-field reach of the watercourse is constant.

Hence, we now simplify the flow in the watercourse into a sequence of steady state, continuous but gradually varied types of flow. For this type of flow, there are established hydraulic descriptions, which are explained below. This enabled us to define relationships between the discharge $Q$ and the gradually changing water depth $h$ in the auxiliary channel for a sequence of discharges.

Cross-section, bottom slope and bed roughness of the auxiliary channel are identical to those of the original edge-of-field watercourse. Compared to the original watercourse the auxiliary channel is extended in both the upstream and downstream directions. In the downstream direction, it is extended down to a freely discharging weir, while in upstream direction it is extended up to the reach with uniform flow. The total distance from the weir to the reach with uniform flow is a function of the discharge in the channel, as well as of the channel characteristics.

For each steady state situation, the flow in the auxiliary channel is continuous, so its discharge is constant and does not vary along the channel length. However, the water depth does change. Travelling in a downstream direction, we start at the constant, *uniform flow* depth, next we enter the reach with gradually changing water depths in the *backwater curve* of the weir, and finally we reach the water depth immediately upstream of the *freely discharging weir*. Figures 7 and 8 present examples of water depth profiles in the auxiliary channel. Figure 8 also illustrates that the length of the channel reach with the backwater curve depends on the size of the discharge.

The backwater curve can only be calculated once its boundary conditions are known, i.e. the uniform flow depth and the water depth in front of the weir. Therefore, we first describe the calculation of the uniform flow depth, then the water depth immediately in front of the weir and only thereafter the calculation of the backwater curve itself. The three calculations are explained in more detail below.

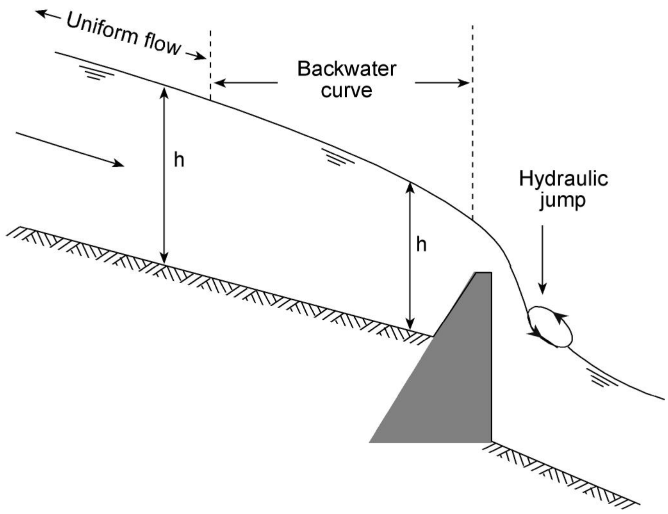



*Figure 7. Example of auxiliary channel with weir. At some distance upstream of the weir, the backwater curve has reached the uniform flow depth. The water depth decreases travelling in a downstream direction towards the weir. Note that the vertical scale is exaggerated compared to the horizontal scale.*

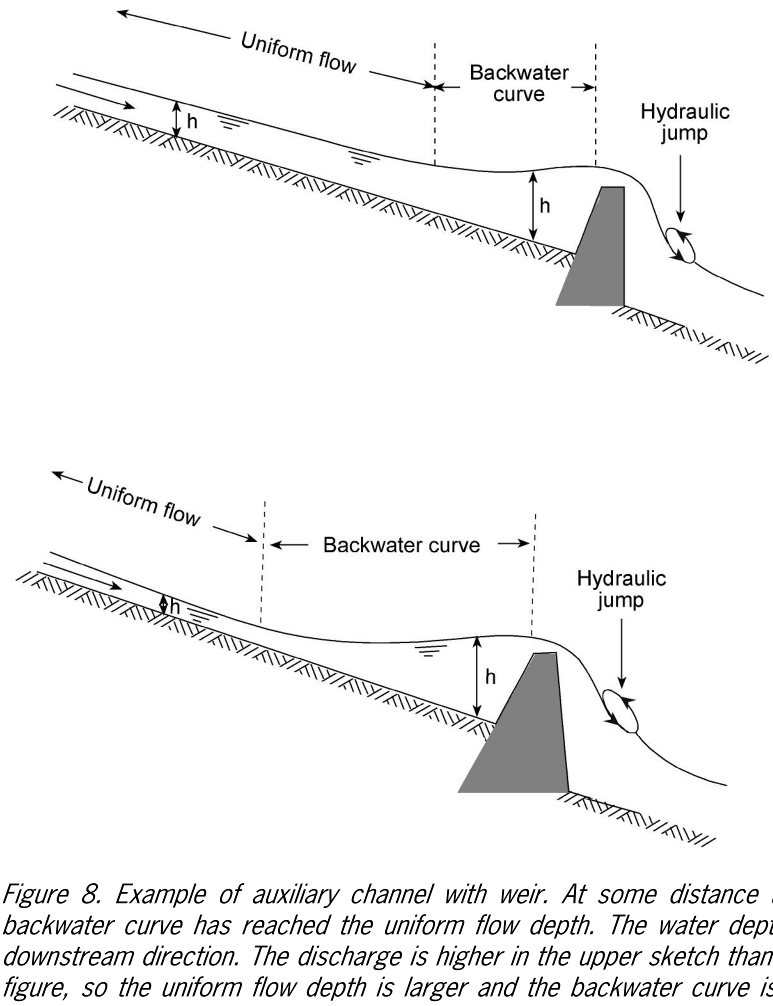



*Figure 8. Example of auxiliary channel with weir. At some distance upstream of the weir, the backwater curve has reached the uniform flow depth. The water depth increases travelling in a downstream direction. The discharge is higher in the upper sketch than in the lower sketch of this figure, so the uniform flow depth is larger and the backwater curve is shorter than in the lower sketch. Note that the vertical scale is exaggerated compared to the horizontal scale.*

### *Water depth for uniform flow*

We assume uniform flow conditions outside the influence of the weir, which is a widely used approximation for continuous flow in open water channels. Uniform flow is characterised by fixed dimensions of the cross-sectional area of flow, a fixed flow velocity (called the uniform flow velocity), a fixed hydraulic gradient and a fixed bed roughness over the entire channel length. The water depth is also fixed at uniform flow, running parallel to the bottom slope of the channel. Hence, uniform flow corresponds to a steady state flow.

For uniform flow, a relation can be derived between the uniform water depth h and the uniform discharge Q. Uniform flow in open water channels corresponds to a simplification of the so-called Saint Venant equation, namely the kinematic wave approximation. The kinematic wave approximation of the one-dimensional Saint Venant equation only considers the effects of gravitation and friction at the wetted perimeter on the water flow; it neglects the effects of wind stress, the Bernoulli term (rate of momentum change by water mass transfer) and the rate of velocity change with respect to time. In open water channels, the kinematic wave approximation of the one-dimensional Saint Venant equation results in the Chézy-Manning equation (Lyklema and Aalderink, 1992).

The Chézy-Manning equation reads (Vennard and Street, 1976):

$$Q = A R^{\frac{2}{3}} k_M \, G^{\frac{1}{2}} \qquad \textit{eq. 18}$$

with

| | | |
|---|---|---|
| $Q$ | = | discharge ($L^3.T^{-1}$) (time) |
| $R$ | = | hydraulic radius of the cross-section (L) (time) |
| $k_M$ | = | Manning coefficient related to the bed roughness ($L^{1/3}.T^{-1}$) (time) |
| $G$ | = | hydraulic gradient, i.e. the ratio of the difference in water level,[8] (relative to a horizontal datum line) to the distance between two locations in the channel (1). |

The hydraulic radius $R$ equals:

$$R = \frac{A}{P} \qquad \textit{eq. 19}$$

and

$$P = b + 2h\sqrt{(s_1^2 + 1)} \qquad \textit{eq. 20}$$

with

| | | |
|---|---|---|
| $P$ | = | wetted perimeter of the channel (L). |

The roughness factor $k_M$ has been defined as a continuous function of the water depth and can be differentiated according to season:

$$k_M = k_{Man,1m} \, h^{\frac{1}{3}} \qquad \textit{eq. 21}$$

with $k_M$ in $m^{1/3}.s^{-1}$ and $h$ in m.

---

[8] Note that the water level refers to the water surface of the water in the channel; for uniform flow, the slope in the water surface equals the slope in the channel bed, i.e. the bottom slope

The parameter $k_{Man,1m}$ represents the Manning coefficient at a water depth of 1 m and may have the following values:

$k_{Man,1m}$ = 23 $s^{-1}$ in summer, assuming vegetation is removed twice a year

$k_{Man,1m}$ = 34 $s^{-1}$ in winter (Werkgroep Herziening Cultuurtechnisch Vademecum, 1988, p. 788). It can also be differentiated according to type of channel.

$k_{Man,1m}$ = 11 $s^{-1}$ for channels representing streams with fast flow, light vegetation and irregular, rippled bed.

$k_{Man,1m}$ = 25 $s^{-1}$ for channels representing ditches with slowly moving water, light vegetation and regular bed.

Substituting the equations 10, 19, 20 and 21 into equation 18 yields the relation between the uniform discharge $Q$ and the uniform flow depth $h$.

### *Water depth immediately in front of the weir*

The layout of the weir determines the relationship between the discharge and the upstream water level over the weir crest. This $Q_{weir}(h_{crest})$ is called a *head-discharge relation*. It is only valid if the weir is freely discharging, allowing the flow across the weir to transit from *subcritical* flow via *critical* flow to *supercritical* flow. This can be seen from the presence of a *hydraulic jump* after the weir, i.e. large flow turbulences in the water, indicating that the supercritical flow regime transits back into the subcritical flow regime. The critical flow state is needed for reasons of simplicity, as (i) there is then only one depth of flow for a given discharge and (ii) the upstream water level is independent of the water level downstream of the weir.

The head-discharge relation reads:

$$Q_{weir} = C w_{crest} h_{crest}^{\frac{3}{2}} \qquad \textit{eq. 22}$$

with

$Q_{weir}$ = rate of discharge across the weir ($L^3.T^{-1}$) (time)

$C$ = discharge coefficient, depending on weir characteristics ($L^{½}$ $T^{-1}$)

$w_{crest}$ = width of weir crest (L)

$h_{crest}$ = upstream water level over the weir crest, also called head (L) (time)

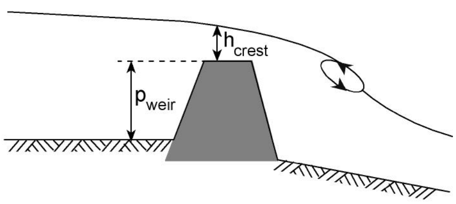



*Figure 9. Water depth at the weir in the watercourse*

The water depth immediately in front of the weir equals

$$h_{weir} = p_{weir} + h_{crest} \qquad \textit{eq. 23}$$

with

$p_{weir}$ = height of weir crest above channel bottom (L)

$h_{weir}$ = water depth immediately in front of weir (L) (time)

Combining equations 22 and 23 results in an equation for the water depth $h_{weir}$, immediately in front of the weir.

### ***Water depth in the backwater curve in front of the weir***

A freely discharging weir in a channel influences the water level upstream of the weir. The weir may cause the water to be drawn down, going towards the weir. Alternatively, the weir may also cause the water to be pushed up. A backwater curve describes the water depth as a function of distance to the weir, with distance starting at the weir and measured in the upstream direction. It continues up to where the flow regime is undisturbed by the weir. We used the Direct Step Method to calculate the backwater curve (e.g. Chow, 1959; Akan, 2006). The Direct Step Method works by dividing the channel into short reaches and carrying the computation forward step by step from the weir in the upstream direction up to where uniform flow prevails. It is based upon the assumption that no energy is lost (e.g. by turbulences) within the channel reach considered (see Eq. 10-40 of Chow (1959) in Appendix 1). The length of the backwater curve depends on the difference in water depth between the water depth in front of the weir and the uniform flow depth upstream.

Appendix 1 presents the details of the Direct Step Method, as described in Chow (1959).
Figures 7 and 8 demonstrate that, when travelling from the weir in the upstream direction, the water depth may increase or decrease, depending on the depth of uniform flow compared to the water depth immediately in front of the weir. In the TOXSWA model, both types of backwater curve may occur.

Summarising, we are now able to describe the entire water depth profile in a watercourse in front of a weir. Starting at the weir and travelling in the upstream direction, the water depth profile consists of (i): the water level above the weir crest defining the water depth immediately in front of the weir, (ii) the backwater curve (from weir to uniform flow) and (iii) uniform flow depth. For a given channel and weir, the water depth profile only depends on the size of the discharge. Hence, we can now obtain the water depth $h$ as a function of distance for each value of discharge $Q$.

### ***FOCUS Surface Water Scenarios***

In the FOCUS Surface Water Scenarios, the ditches and streams have a rectangular cross-section of 1 m. Their minimum water depth is 0.30 m. All FOCUS ditches have a bottom slope of 0.1‰, while the bottom slope for the FOCUS streams is 1‰ (D1, D2, D4, R1 and R4) or 2‰ (D5, R2 and R3). The Manning coefficient for bed roughness at 1 m water depth $k_{Man,1m}$ has a value of 11 $s^{-1}$ for FOCUS streams and 25 $s^{-1}$ for FOCUS ditches.

The auxiliary channels of the FOCUS ditches and streams have cross-sections, bottom slopes and bed roughness values identical to those described above. For FOCUS ditches, the discharge varies between approximately 0.12 and 820 $m^3$/d, and their uniform flow depth ranges from 2 mm to 22 cm. In the auxiliary channels of FOCUS streams, the discharge varies between approximately 0.60 and 44830 $m^3$/d, resulting in uniform flow depths of 5 mm to 2.12 m (for a bottom slope of 1‰) or between 74.2 and 30760 $m^3$/d, resulting in uniform flow depths of 4 cm to 1.30 m (for a bottom slope of 2‰). All values refer to the winter cereal crop in the D-scenarios and maize in the R-scenarios.

For the FOCUS ditches, the weir in the auxiliary channel has a crest height of 0.4 m and a crest width of 0.50 m. The corresponding values for the FOCUS streams are 0.5 m for crest height as well as crest width. The discharge coefficient of the weirs equals 1.7 $m^{½}.s^{-1}$. (Ministère des Relations Extérieures, Coopération et Développement, 1984). The maximum head over the weir crest is 5 cm for the auxiliary channels of the ditches and 72 or 56 cm for the auxiliary channels of streams (for 1‰ and 2‰ bottom slopes, respectively).

The backwater curves are generally a few tens up to a few hundreds of metres long. Appendix 2 presents examples of backwater curves in FOCUS ditches and streams.

# 4 Boundary conditions and initial condition

## 4.1 Ponds

The inflow in the pond at $x$ = 0, $Q_{pond,0}$, consists of a small base flow. Hence, the upper boundary condition of the water balance for the pond is defined as:

for $t \geq 0$ and $x = 0$

$$Q_{pond,0} = Q_{base} \qquad \textit{eq. 24}$$

with

$Q_{pond,0}$ = discharge or volumic rate of water at the upper boundary of the pond (at $x$ = 0) ($L^3\ T^{-1}$)

$Q_{base}$ = discharge of the base flow ($L^3\ T^{-1}$)

The lower boundary condition at $x = l_{pond}$ consists of the outflow across the weir, so:

for $t \geq 0$ and $x = l_{pond}$

$$Q_{pond,l_{pond}} = Q_{weir,pond} \qquad \textit{eq. 25}$$

with

$Q_{pond,l\_pond}$ = discharge or volumic rate of water at the lower boundary of the pond (at $x = l_{pond}$) ($L^3\ T^{-1}$) (time)

Initially, we assume there is only base flow, so the initial condition reads:

for $t = 0$ and $x > 0$

$$Q_{pond,l_{pond}} = Q_{base} \qquad \textit{eq. 26}$$

resulting in the initial pond volume (eqns 6, 16 and 17)

$$V_{pond,initial} = b_{pond}\, l_{pond} \left( p_{weir} + \left( \frac{Q_{base}}{C_{pond}\, w_{crest,pond}} \right)^{\frac{2}{3}} \right) \qquad \textit{eq. 27}$$

## 4.2 Watercourses, including FOCUS ditches and streams

The discharge in the edge-of-field watercourse at $x$ = 0, $Q_0$, is composed of a small base flow from the upstream catchment and a variable excess water flow from the upstream catchment. Hence, the upper boundary condition of the water conservation equation is defined as:

for $t \geq 0$ and $x = 0$

$$Q_{x=0} = Q_{base} + q_{rodr}\, A_{up} \qquad \textit{eq. 28}$$

with

$Q_{x=0}$ = discharge or volumic rate of water at the upper boundary of the watercourse (at $x$ = 0) ($L^3$ $T^{-1}$) (time)

$Q_{base}$ = discharge of the base flow delivered by the upstream catchment ($L^3$ $T^{-1}$) (time)

$A_{up}$ = size of the upstream catchment area ($L^2$)

(For $q_{rodn}$, see eq 15.)

It is for this discharge $Q_{x=0}$ that the water depth in the watercourse is calculated, so $Q_{x=0}$ results in $h_{x=0}$. Hence, the following condition also holds at the upper boundary:
for t ≥ 0 and x = 0

$$h_{x=0} = h(Q_{x=0}) \qquad eq.\ 29$$

This water depth $h_{x=0}$ corresponds to the water depth in the water depth profile h(x) of the auxiliary channel at a selected, fixed distance upstream of the weir, for a discharge in the auxiliary channel equalling the discharge of the edge-of-field watercourse at x=0:

$$Q_{aux.ch} = Q_{x=0} \qquad eq.\ 30$$

with

$Q_{aux.ch}$ = discharge in the auxiliary channel, function of time only ($L^3.T^{-1}$) (time)

$Q_{x=0}$ = discharge in the original watercourse at distance $x$ = 0 ($L^3.T^{-1}$) (time)

The fixed distance is determined by e.g. the minimum required water depth in the edge-of-field watercourse. We thus obtain a unique relationship between the discharge $Q_{x=0}$ and the water depth $h$ in the original edge-of-field watercourse, based upon a simplified hydraulic description of flow.

In section 2.4 we explained that we had simplified the water flow in the edge-of-field watercourse by assuming that the water depth is constant in the direction of flow (i.e. it only varies in time). Hence, if $h_{x=0}$ is known, $h_{x=l}$ is also known, so the lower boundary condition for the edge-of-field watercourse at $x = l$ reads:
for $t \geq 0$ and $x = l$

$$h_{x=l} = h_{x=0} \qquad eq.\ 31$$

Initially, we assume there is only base flow, so the initial boundary condition reads:
for $t = 0$ and $x > 0$

$$Q = Q_{base} \qquad eq.\ 32$$

For the FOCUS Surface Water Scenarios, the distance at which the water depth is selected in the auxiliary channel differs between the scenarios, being 1000 m upstream of the weir for all ditches, 200 m for the streams of the D1, D2 and D4 scenarios and 110 m for the streams of the D5, R1, R2, R3 and R4 scenarios. Discharges range from 0.001 to 12.8 L/s in FOCUS ditches (corresponding to flow velocities of up to approximately 3000 m/d), and from 0.007 to 503 L/s in FOCUS streams (corresponding to flow velocities of up to approximately 29000 m/d). These discharges result in water depths varying between 0.30 and 0.36 m for FOCUS ditches and between 0.29 and 1.51 m for FOCUS streams. Appendix 3 presents a few examples of water depth as a function of $Q_{in}$, viz. D2 and D6 ditches and D2 and R4 streams. As expected, the graphs indicate that there is a unique relation between $Q_{x=0}$ and $h$.

# 5 Numerical solution of the water conservation equations

## 5.1 Introduction

The water conservation equations have been solved numerically with the aid of the finite-difference method. For this purpose, a rectangular grid of points in the water layer was defined in the (*x,t*) plane, numbered $i$ = 1, 2, 3, ……. along the $x$ axis and $j$ = 1, 2 ,3 ,…….. along the $t$ axis. The $x$ axis was assumed to be positive in the direction of dominant flow. $\Delta x_i$ was defined as the length of a segment around point $i$, while $\Delta t$ was defined as the time step (Figure 10). Water flow was described with the aid of the water depth at a grid point and the flow velocity or discharge through an interface. The upper boundary of the water subsystem is located at $x$ = 0 and the lower boundary at the end value of $x$.

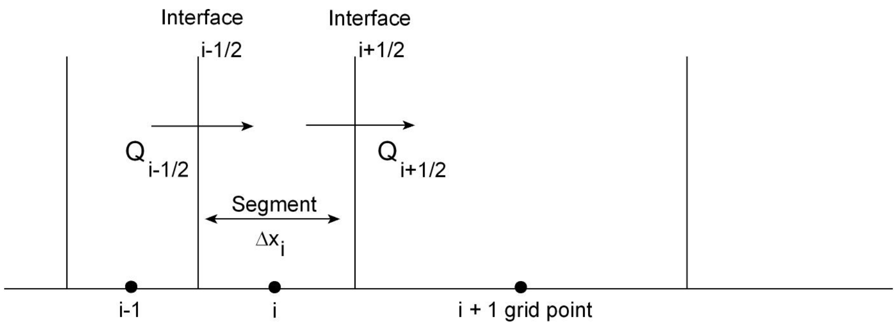



*Figure 10. Outline defining the discretisation of the x-axis (water layer)*

## 5.2 Ponds

Only the derivatives with respect to time remained in the water conservation equation for the pond (eq 5). This means that the numerical solution considers only the temporal derivative of $V_{pond}$. We used the finite-difference solution scheme in its explicit form to solve the water conservation equation. The explicit solution implies that the right-hand term was evaluated at time $j$:

$$\left(Q^j{}_{pond,o} - Q^j{}_{pond,l_{pond}}\right) + \Phi^j{}_{pond}\, l_{pond} + \left(N^j + E^j\right) l_{pond}\, b_{pond} - S^j P_{z=o}\, l_{pond}$$

The left-hand term was approximated as:

$$\frac{dV_{pond}}{dt} \approx \frac{V^{j+1}_{pond} - V^{j}_{pond}}{\Delta t} = \frac{\left(h^{j+1}_{pond} - h^{j}_{pond}\right) b_{pond}\, l_{pond}}{\Delta t}$$

Hence, the water conservation equation can be approximated by

$$\frac{\left(h_{pond}^{j+1}-h_{pond}^{j}\right)b_{pond}\,l_{pond}}{\Delta t}=\left(Q^{j}{}_{pond,o}-Q^{j}{}_{pond,l_{pond}}\right)+\Phi^{j}{}_{pond}\,l_{pond}+\left(N^{j}+E^{j}\right)l_{pond}\,b_{pond}-S^{j}P_{z=o}\,l_{pond}\Leftrightarrow$$

$$h_{pond}^{j+1}=h_{pond}^{j}+\Delta t\left(\frac{\left(Q^{j}{}_{pond,o}-Q^{j}{}_{pond,l_{pond}}\right)}{b_{pond}\,l_{pond}}+\frac{\Phi_{pond}^{j}}{b_{pond}}+N^{j}+E^{j}-\frac{S^{j}P_{z=o}}{b_{pond}}\right) \qquad \textit{eq. 33}$$

The water depth at the next time step, *j+1*, can thus be calculated from the inflow, excess water from the contributing area and the outflow at time step *j*.

This was implemented in the TOXSWA model.

## 5.3 Watercourses

In section 3.3 we explained how we simplified the flow in the watercourse into a sequence of steady state, continuous but gradually varied types of flow, which was simplified further into a sequence of steady state and continuous flows with a constant water depth over its edge-of-field reach. For the edge-of-field watercourse, the water conservation equation can thus be solved for a water depth *h*, constant over distance *x*, and flows *Q* and other fluxes varying in time.

The water conservation equation was solved with the aid of the finite-difference solution scheme, expressed in its central explicit form. The water flux terms *Φ*, *N*, *E* and *S,* the water depth *h* and the water surface width *O* are constant over distance *x* in the watercourse, but vary in time. For the numerical solution, the spatial derivatives and the terms *Φ*, *N*, *E*, *S, h* and *O* are evaluated at time *j*, so the right-hand term in eq. 9 is:

$$-\left(\frac{\partial Q_x}{\partial x}\right)_i^j+\Phi^j+N^j\cdot O^j+E^j\cdot O^j-S^j\cdot P_{z=0}\approx$$
$$-\left(\frac{Q^j_{i+\frac{1}{2}}-Q^j_{i-\frac{1}{2}}}{\Delta x_i}\right)+\Phi^j+N^j\cdot O^j+E^j\cdot O^j-S^j\cdot P_{z=0}$$

The water depth *h* is constant over distance *x*, so the cross-sectional area of flow *A* is also constant over distance *x*. The left-hand term of the water conservation equation is approximated as:

$$\frac{\partial A}{\partial t}\approx\frac{A_i^{j+1}-A_i^j}{\Delta t}\approx\frac{A^{j+1}-A^j}{\Delta t}$$

Hence, the entire water conservation equation can now be approximated by:

$$\frac{A^{j+1}-A^j}{\Delta t}=-\frac{Q^j_{i+\frac{1}{2}}-Q^j_{i-\frac{1}{2}}}{\Delta x_i}+\Phi^j+N^j\cdot O^j+E^j\cdot O^j-S^j\cdot P_{z=0} \qquad \textit{eq. 34}$$

The terms $\Phi$, $N$, $E$ and $S$ are defined as a function of time outside the TOXSWA model, i.e. they are known at all times $j$. The same holds for the term $Q_{x=0}$, because the terms $Q_{base}$ and $q_{rodr}$ are also defined as a function of time outside the TOXSWA model. Hence, $Q^{j}_{x=0}$ and $Q^{j+1}_{x=0}$ are both known.

The discharge at $x = 0$, $Q^{j}_{x=0}$, determines the water depth $h$, which in its turn determines the water surface width $O$ (eq 11). Hence, $Q^{j}_{x=0}$ determines $h^{j}$ and $O^{j}$. Because $Q^{j+1}_{x=0}$ is also known, $h^{j+1}$ and also $A^{j+1}$ are known. This means that rewriting (eq 34) and starting at $i = 0$ allows $Q^{j}_{i+\frac{1}{2}}$ to be calculated for all $i$, $j$ and $j+1$ by

$$Q^{j}_{i+\frac{1}{2}} = Q^{j}_{i-\frac{1}{2}} + \Delta x_i \left( \frac{A^{j} - A^{j+1}}{\Delta t} + \Phi^{j} + N^{j} \cdot O^{j} + E^{j} \cdot O^{j} - S^{j} \cdot P_{z=0} \right) \qquad \textit{eq. 35}$$

This was implemented in the TOXSWA model.

# 6 Verification

## 6.1 Introduction

After a computer program has been written, it must be verified. Verification is defined as the examination of the numerical technique in the model to ascertain that it truly represents the mathematical model and that there are no inherent numerical problems in obtaining a solution. This also implies a check on errors in the code (programming bugs). Adriaanse (1996) operationalized the verification of the TOXSWA model by applying the three notions of convergence, stability and consistency. The condition of convergence states that when the finite-difference grid is refined, the truncation errors go to zero. Stability concerns the unstable growth or stable decay of errors in the arithmetic operations required to solve the finite-difference equations. Consistency is the requirement that refining the finite-difference model makes the truncation errors decrease to zero, but also that the finite-difference model approximates the desired partial differential equation and not some other partial differential equation. In Adriaanse (1996) these three notions were evaluated for the numerical solution of the mass conservation equations for the water and sediment layers of a watercourse with constant flow conditions. For the simple and straightforward numerical solutions of the water conservation equations for the pond and the watercourse in this report, we evaluated only the convergence, and formulated a restriction on the time step.

***Convergence***
A solution obtained with by reducing the time and space steps by e.g. a factor of 10 should differ only slightly from the solution obtained with the original time and space steps. This means that in this case the truncation errors are so small that the numerical equations yield nearly the same solution.

***Restriction on selection of time step***
The solution of the water conservation equations for the two types of water body needs to be stable, that is, the errors in the arithmetic operations required to solve the finite-difference equations should be bounded. One of the requirements for stability here is that the water depth in the numerical solution should be positive. This leads to a restriction on the selection of possible time steps.

## 6.2 Ponds

***Convergence***
Since the pond is an ideally mixed reservoir, there is only one segment in space. Hence, the convergence of the numerical solution needs to be checked for the time step only. We selected two ponds with the greatest variations in water flow, viz. the FOCUS D5 and R1 ponds (weather year 1984, used for pesticide applications from March to May) and solved the water conservation equation with a time step reduced by a factor of 6, i.e., 100 s instead of the usual 600 s. Appendix 4 presents graphs of the water depths and discharges across the weir at the pond outlet. The first set of graphs presents the water depth and discharge of the D5 pond. Correspondence between the plots obtained with the 600 s time step and those obtained with the 100 s time step is good, both for the water depth and for the discharge, including the plots where we zoomed in on selected short periods. This is also the case for the next set of graphs for the R1 pond. Only in the water depth plot for days 320 to 340 slight

differences between the two numerical solutions visible, but these are minor. In all, therefore, correspondence between the two numerical solutions is good and we conclude that the numerical solution of the water conservation equation in TOXSWA is sufficiently convergent for ponds.

Restriction on time step.

The numerical solution of the pond equation (eq. 33) reads:

$$h_{pond}^{j+1} = h_{pond}^{j} + \Delta t \left( \frac{\left( Q^{j}{}_{pond,o} - Q^{j}{}_{pond,l_{pond}} \right)}{b_{pond}\, l_{pond}} + \frac{\Phi_{pond}^{j}}{b_{pond}} + N^{j} + E^{j} - \frac{S^{j} P_{z=o}}{b_{pond}} \right)$$

The terms $h_{pond}^{j}$ and $h_{pond}^{j+1}$ must be positive. If the large term between brackets is positive, then $\Delta t$ needs to be positive, so this imposes no restriction on the selection of $\Delta t$, as it is always greater than a negative value.

If the large term between brackets is negative, however, then

$$\Delta t \leq \frac{-h_{pond}^{j}}{\left( \frac{\left( Q^{j}{}_{pond,o} - Q^{j}{}_{pond,l_{pond}} \right)}{b_{pond}\, l_{pond}} + \frac{\Phi_{pond}^{j}}{b_{pond}} + N^{j} + E^{j} - \frac{S^{j} P_{z=o}}{b_{pond}} \right)} \qquad \textit{eq. 36}$$

This second condition does impose a real restriction on the selection of $\Delta t$.

## 6.3 Watercourses

***Convergence***

We checked the convergence of the numerical solution of the water conservation equation for two ditches and two streams. We selected the D2 ditch and stream, because the heavy clay soil of the D2 scenario produces highly variable drainage fluxes that enter the watercourse. Next, we selected the D6 ditch and the R4 stream (weather year 1985, used for pesticide applications from June to September) because they receive the highest excess drainage and runoff fluxes of all FOCUS scenarios. The current numerical solution uses 10 segments of 10 m each for the FOCUS ditch and 20 segments of 5 m each for the FOCUS stream. We repeated the calculations with segments reduced by a factor of 5, i.e. 2 m for the FOCUS D2 and D6 ditches and 1 m for the FOCUS D2 and R4 streams. We also shortened the calculation time step to 100 s to solve the water conservation equation, instead of the fixed 600 s TOXSWA uses. Appendix 4 presents the results of these calculations. Correspondence between the two numerical solutions is good In all four cases. Hence, the numerical solution of the water conservation equation for the watercourse is sufficiently convergent for the calculation of both the water depth and the discharge as a function of time.

### *Restriction on time step*

The numerical solution of the water conservation equation of the watercourse (eq. 34) reads:

$$\frac{A^{j+1} - A^{j}}{\Delta t} = -\frac{Q^{j}_{i+\frac{1}{2}} - Q^{j}_{i-\frac{1}{2}}}{\Delta x_i} + \Phi^{j} + N^{j} \cdot O^{j} + E^{j} \cdot O^{j} - S^{j} \cdot P_{z=0} \Leftrightarrow$$

$$A^{j+1} = A^{j} + \Delta t\left(-\frac{Q^{j}_{i+\frac{1}{2}} - Q^{j}_{i-\frac{1}{2}}}{\Delta x_i} + \Phi^{j} + N^{j} \cdot O^{j} + E^{j} \cdot O^{j} - S^{j} \cdot P_{z=0}\right)$$

The terms $A^j$ and $A^{j+1}_i$ must be positive. If the large term between brackets is positive, then $\Delta t$ needs to be positive, so this imposes no restriction on the selection of $\Delta t$, as it is always greater than a negative value.

If however $\left(-\frac{Q^{j}_{i+\frac{1}{2}} - Q^{j}_{i-\frac{1}{2}}}{\Delta x_i} + \Phi^{j} + N^{j} \cdot O^{j} + E^{j} \cdot O^{j} - S^{j} \cdot P_{z=0}\right) < 0$

then

$$\Delta t < \frac{-A^{j}}{\left(-\frac{Q^{j}_{i+\frac{1}{2}} - Q^{j}_{i-\frac{1}{2}}}{\Delta x_i} + \Phi^{j} + N^{j} \cdot O^{j} + E^{j} \cdot O^{j} - S^{j} \cdot P_{z=0}\right)} \qquad \textit{eq. 37}$$

The condition in eq. 37 imposes a restriction on the selection of $\Delta t$.

# 7 Example simulations

Appendices 5 and 2 present elements of the water balance as a function of time for the example simulations, the R1 pond, D3 ditch, D1 stream and R2 stream.

The first set of graphs of Appendix 5 present the R1 pond (weather year for spring applications), showing the surface runoff flux of the contributing area (4500 $m^2$), the pond outflow, its water depth and the hydraulic residence time. The R1 pond is situated in a silty loam soil. The incoming runoff fluxes are event-driven and may be as high as approximately 1.4 mm/h. The response of the pond outflow is rapid, but remains small, up to approximately 1.3 L/s. Water level rise is negligible, a few centimetres at most.

The hydraulic residence time is defined as

$$\tau = \frac{V}{Q} \qquad \textit{eq. 38}$$

in which

$\tau$ = hydraulic residence time (T) (time)
V = volume of water body considered ($L^3$) (time)
Q = discharge flowing out of water body ($L^3.T^{-1}$) (time)

The instantaneous as well as the average hydraulic residence time are indicated in the graph, using the discharge for the entire month for the latter. The hydraulic residence time is used by FOCUS to characterise the dynamics of flow in a water body and intends to give an indication of the relevant time during which a pesticide mass that has entered the water may be found in the water body.

In the R1 pond, the average hydraulic residence time is between 120 and 150 d, while instantaneous values may be as low as approximately 20 d.

The second set of graphs of Appendix 5 shows the D3 ditch water balance elements. The D3 ditch is located in sandy soil and only involves drainage through the soil matrix, so no rapid macropore flow occurs. The drainage fluxes of the upper graph form a relatively continuous flow, unlike the runoff fluxes of e.g. the R1 pond, or the drainage fluxes of the D1 stream (next set of graphs). The D3 drainage fluxes range from approximately 0.01 to 0.09 mm/h. The inflow across the upper boundary and the ditch outflow reflect the dynamics of incoming drainage fluxes: the inflow ranges from approximately 0.1 to 0.5 L/s, while the outflow may be as high as approximately 0.7 L/s. The inflow consists of a small constant base flow (0.001 L/s) plus the drainage fluxes from a 1 ha area, while the outflow consists of drainage fluxes from an additional 2 ha which have flowed into the ditch. The water depth in the ditch varies only by about 0.5 cm, between 0.30 and 0.31 m. Monthly average hydraulic residence times are approximately 0.5 to 5 d and instantaneous residence times vary little from these values. Thus, compared to the R1 pond, the water has left the D3 ditch much more rapidly.

The first diagram in Appendix 2 shows the backwater curve in the auxiliary channel of the D3 ditch. Minimum and maximum discharges at $x = 0$ in D3 ditch are 0.08 and 0.71 L/s. These discharges result in water levels on the weir crest of 0.2 and 28 cm and water depths of 40.2 and 68 cm immediately in front of the weir, respectively. The diagram shows that the water depth decreases as one moves in the upstream direction; at 1000 m upstream of the weir, the difference in water level between the minimal and maximal discharge has been reduced from 28 cm on the weir crest to 1 cm at the upper boundary of the auxiliary channel. Calculation of the backwater curves was explained in section 3.3.

The D1 stream is presented in the third set of graphs of Appendix 5. The D1 stream has a more dynamic behaviour than the D3 ditch, receiving only matrix flow drainage fluxes. The D1 stream is situated in a silty clay soil and also receives the more rainfall event-driven drainage fluxes through macropores. Drainage fluxes may be as high as approximately 0.5 mm/h. Again, the ditch inflow across the upper boundary and the ditch outflow closely reflect the drainage flux dynamics, as they rise to approximately 130 L/s. Water depth variations in the ditch are large, ranging from 30 to 85 cm. The monthly average hydraulic residence times reflect the dynamic behaviour, ranging from a few hours to approximately 1 d. Instantaneous residence times may be as low as 1 h or less.

The second diagram in Appendix 2 shows the backwater curve in the auxiliary channel of the D1 stream. Minimum and maximum discharges at $x = 0$ in the D1 stream are 0.38 and 131 L/s. These discharges result in water levels on the weir crest of 0.6 and 29 cm and water depths of 50.6 and 79 cm immediately in front of the weir, respectively. The diagram shows that as one moves in the upstream direction, the water depth may decrease (M1 type of backwater curve) or increase (M2 type); in the latter case, the backwater curve is a so-called drawdown curve. At 200 m upstream of the weir, the difference in water level between the minimal and maximal discharge has increased from 29 cm on the weir crest to 51 cm at the upper boundary of the auxiliary channel.

The R2 stream is presented in the fourth and final set of water balance element graphs in Appendix 5. The R2 stream is situated in a sandy loamy soil area, which receives a high amount of annual rainfall, approximately 1400 mm. Runoff fluxes may be as high as 1.2 mm/h. The stream outflow again closely reflects the runoff fluxes from the 100 ha upstream catchment and the adjacent 1 ha field. Stream discharge may be as high as approximately 350 L/s and stream depth as high as approximately 1.2 m. The incoming water fluxes, discharges and water depth in the R2 stream change more abruptly than those in the D1 stream, reflecting the fact that drainage fluxes partly consist of slowly increasing and decreasing matrix flow, while runoff is more of an on/off process. Monthly average hydraulic residence times are a few hours, while instantaneous residence times may be as low as a few minutes.

The third diagram in Appendix 2 shows the backwater curve in the auxiliary channel of the R2 stream. Minimum and maximum discharges at $x = 0$ in R2 stream are 3.24 and 350 L/s. These discharges result in water levels on the weir crest of 2 and 55 cm and water depths of 52 and 105 cm immediately in front of the weir, respectively. The diagram shows that as one moves in the upstream direction, the water depth may decrease (M1 type of backwater curve) or increase (M2 type, drawdown curve). At 110 m upstream of the weir, the difference in water level between the minimal and maximal discharges has increased from 53 cm on the weir crest to 86 cm at the upper boundary of the auxiliary channel.

For a description of the water balance elements and other hydrological characteristics of all FOCUS Surface Water Scenarios, we refer to FOCUS (2001), especially Appendix F and sections 4.3 and 4.4.

# 8 Conclusions and recommendations

## 8.1 Conclusions

The TOXSWA model has been expanded with a transient flow module, which was developed in the 1999-2001 period to support the use of the FOCUS Surface Water Scenarios in the EU registration procedure. TOXSWA can now simulate varying discharges and water depths for edge-of-field ponds and watercourses fed by excess water fluxes from an adjacent area or small upstream catchment, with weirs located at the pond outflow or at a downstream location in the watercourse maintaining minimum water levels.

Up to now, the transient flow module has only been parameterized and tested for the layout of the 15 water bodies featured in the 10 standard FOCUS Surface Water Scenarios. The excess runoff water fluxes are calculated by the PRZM model, while the excess drainage fluxes are calculated by the MACRO model. As the 10 FOCUS scenarios represent a large area of agriculture in the European Union with a range of climate, topography, soil type and crop and agricultural management practices, the excess water fluxes and the flow in the FOCUS ponds, ditches and streams cover a relatively broad range of conditions (Appendix F, FOCUS, 2001).

Looking back it was unnecessary to introduce the simplification of a constant water depth for the entire reach of the edge-of-field watercourse. For each $Q$ at $x = 0$ and for all times, the entire water depth profile is calculated in the auxiliary channel anyway, and this profile can simply be used in the numerical solution of the water conservation equation of the edge-of-field watercourse.

A limited verification of the transient flow module was undertaken by comparing discharge and water depth output values obtained using smaller time and space steps with output values obtained using the original time and space steps. It shows that the numerical solutions for the water conservation equations of the pond and the watercourse are sufficiently convergent.

A number of example simulations have been presented, which demonstrate the model's ability to handle incoming excess water fluxes at an hourly resolution and to simulate an immediate response in water depth and discharge in the pond or watercourse.

## 8.2 Recommendations

We recommend incorporating the water balance terms of precipitation, evaporation and seepage in the TOXSWA computer program. This will result in more realistic water level fluctuations, especially in ponds and ditches with low base flows. Note that the inclusion of precipitation, evaporation and seepage may lead to an additional condition for the base flow (e.g. minimum value), if the minimum water depth in the watercourse needs to be maintained throughout the entire simulation period.

We strongly recommend dropping the assumption of a constant water depth $h(x)$ in the watercourse as (i) it is unnecessary, (ii) it is unrealistic (especially in FOCUS streams with high discharges) and (iii) it forms an additional condition that may prevent the numerical solution of the water balance conservation equation from correctly representing the water flow ($Q_{x=l}$ may become negative, which is incorrect if $P=E=S=0$).

Suggestions have been made to replace the current explicit numerical solution of the water conservation equation for watercourses by another classical method for solving implicit functions, viz. root finding functions, such as e.g. Brent's algorithm (function zbrent of Press *et al*, 1992).

Another option might be to consider the exact integration of the two equations (water conservation equation and *Q(h)* relation) for watercourses, for instance using the Crank-Nicholson numerical solution scheme, instead of the present approximation, which makes use of an auxiliary channel. The present approach uses two successive assumptions, namely uniform water depth (in the edge-of-field watercourse and its water conservation equation) and uniform water flux (in the *Q(h)* relation for the backwater curve in the auxiliary channel), and it is not entirely clear how reliable the results of this procedure are. We suggest dropping both assumptions and implementing a mathematical description for a gradually varied flow in front of a weir that is also spatially varied, i.e. where water may enter and leave a flow along its course.

The verification of the numerical solutions of the water conservation equations for the pond and the watercourse can be improved, for instance by (i) checking that all water that enters can be traced at every moment with a defined degree of error in the water balance or (ii) comparing the numerical solution of the water conservation equations with analytical solutions. Analytical solutions for ponds have been derived for a static test and for a pond with no inflow converging from an initially raised water level to its equilibrium water level (pers. comm. J. Molenaar, Biometris, Wageningen UR).

In 1998, the TOXSWA model was subjected to a sensitivity analysis (Westein *et al*, 1998). We recommend a new sensitivity analysis for the current FOCUS version of the TOXSWA model, to identify which input parameters contribute most to the variation in model output (notably the pesticide concentration output) under transient flow conditions. In addition to this sensitivity analysis, there is also a need for an uncertainty analysis to identify the influence of the input uncertainty on the output uncertainty for specific situations, such as the FOCUS scenarios.

Finally, we recommend testing the transient flow module of TOXSWA against field measurements in ponds or small watercourses located at the downstream end of small catchments.

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# Appendix 1 Direct Step method to calculate the backwater curve from Chow, (1959)

**10-3. The Direct Step Method.** In general, a step method is characterized by dividing the channel into short reaches and carrying the computation step by step from one end of the reach to the other. There is a great variety of step methods. Some methods appear superior to others in certain respects, but no one method has been found to be the best in all

[1] If $S_0 = 0$, then $Q_0 = 0$, $Q/Q_0 = \infty$, and the varied-flow functions become meaningless. If $S_0$ is negative, Eq. (10-30) shows that $Q_0{}^2$ is negative. Since the actual discharge $Q$ must be positive, $(Q/Q_0)^2$ becomes negative. Thus, the integration procedure must be done for negative values of $(Q/Q_0)^2$ in the two varied-flow functions.

applications. The direct step method[1] is a simple step method applicable to prismatic channels.

Figure 10-6 illustrates a short channel reach of length $\Delta x$. Equating the total heads at the two end sections 1 and 2, the following may be written:

$$S_0\,\Delta x + y_1 + \alpha_1 \frac{V_1^2}{2g} = y_2 + \alpha_2 \frac{V_2^2}{2g} + S_f\,\Delta x \qquad (10\text{-}40)$$

Solving for $\Delta x$,

$$\Delta x = \frac{E_2 - E_1}{S_0 - S_f} = \frac{\Delta E}{S_0 - S_f} \qquad (10\text{-}41)$$

where $E$ is the specific energy or, assuming $\alpha_1 = \alpha_2 = \alpha$,

$$E = y + \alpha \frac{V^2}{2g} \qquad (10\text{-}42)$$

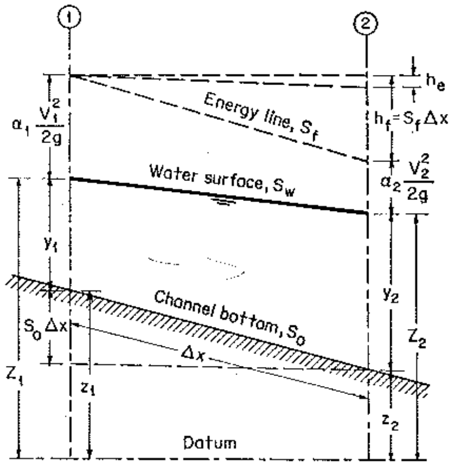



FIG. 10-6. A channel reach for the derivation of step methods.

In the above equations, $y$ is the depth of flow, $V$ is the mean velocity, $\alpha$ is the energy coefficient, $S_0$ is the bottom slope, and $S_f$ is the friction slope. The average value of $S_f$ is denoted by $\bar{S}_f$. When the Manning formula is used, the friction slope is expressed by

$$S_f = \frac{n^2 V^2}{2.22 R^{4/3}} \qquad (9\text{-}8)$$

The direct step method is based on Eq. (10-41), as may be illustrated by the following example:

**Example 10-7.** Compute the flow profile required in Example 10-1 by the direct step method.

*Solution.* With the data given in Example 10-1, the step computations are carried out as shown in Table 10-4. The values in each column of the table are explained as follows:

Col. 1. Depth of flow in ft, arbitrarily assigned from 5.00 to 3.40 ft
Col. 2. Water area in ft² corresponding to the depth $y$ in col. 1
Col. 3. Hydraulic radius in ft corresponding to $y$ in col. 1
Col. 4. Four-thirds power of the hydraulic radius
Col. 5. Mean velocity in fps obtained by dividing 400 cfs by the water area in col. 2
Col. 6. Velocity head in ft
Col. 7. Specific energy in ft obtained by adding the velocity head in col. 6 to the depth of flow in col. 1

[1] First suggested by the Polish engineer Charnomskiĭ [22] in 1914 and then by Husted [23] in 1924.

Col. 8. Change of specific energy in ft, equal to the difference between the $E$ value in col. 7 and that of the previous step

Col. 9. Friction slope computed by Eq. (9-8) with $n = 0.025$ and with $V$ as given in col. 5 and $R^{2/3}$ in col. 4

Col. 10. Average friction slope between the steps, equal to the arithmetic mean of the friction slope just computed in col. 9 and that of the previous step

Col. 11. Difference between the bottom slope 0.0016 and the average friction slope

Col. 12. Length of the reach in ft between the consecutive steps, computed by Eq. (10-41) or by dividing the value of $\Delta E$ in col. 8 by the value in col. 11

Col. 13. Distance from the section under consideration to the dam site. This is equal to the cumulative sum of the values in col. 12 computed for previous steps.

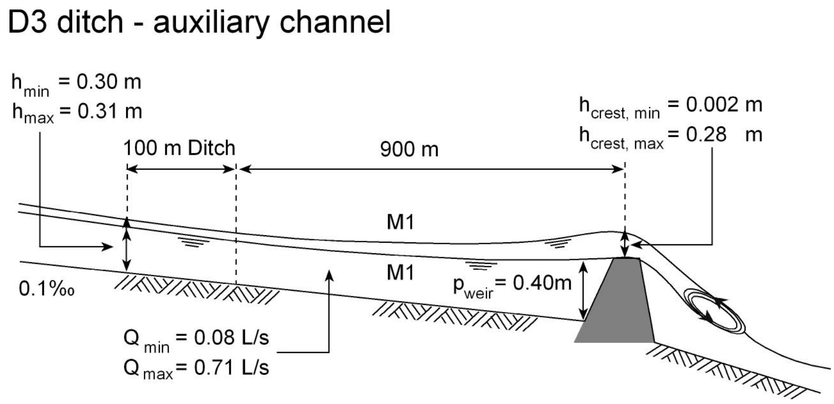
The flow profile thus computed is practically identical with that obtained by graphical integration (Fig. 10-3).

Table 10-4. Computation of the Flow Profile by the Direct Step Method for Example 10-7

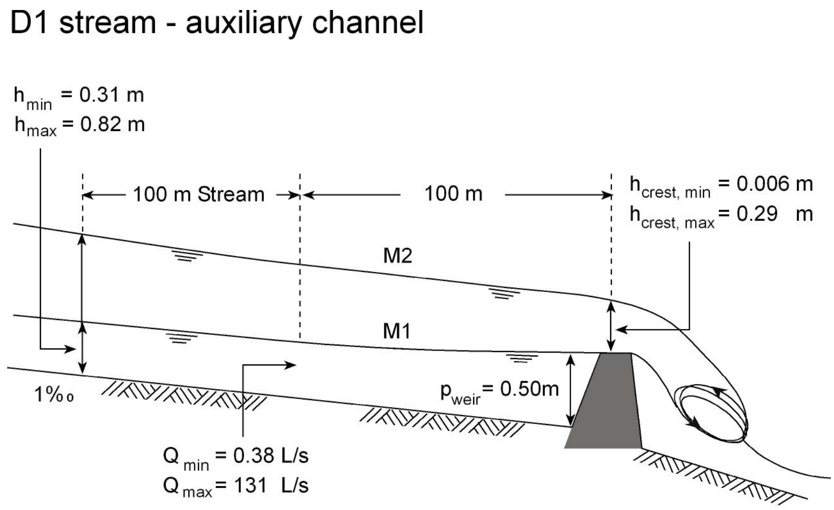
$Q$ = 400 cfs $n$ = 0.025 $S_0$ = 0.0016 $\alpha$ = 1.10 $y_c$ = 2.22 ft $y_n$ = 3.36 ft

| $y$ (1) | $A$ (2) | $R$ (3) | $R^{4/3}$ (4) | $V$ (5) | $\alpha V^2/2g$ (6) | $E$ (7) | $\Delta E$ (8) | $S_f$ (9) | $\bar{S}_f$ (10) | $S_0 - \bar{S}_f$ (11) | $\Delta x$ (12) | $x$ (13) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 5.00 | 150.00 | 3.54 | 5.40 | 2.667 | 0.1217 | 5.1217 | ...... | 0.000370 | | | | |
| 4.80 | 142.08 | 3.43 | 5.17 | 2.819 | 0.1356 | 4.9356 | 0.1861 | 0.000433 | 0.000402 | 0.001198 | 155 | 155 |
| 4.60 | 134.32 | 3.31 | 4.94 | 2.979 | 0.1517 | 4.7517 | 0.1839 | 0.000507 | 0.000470 | 0.001130 | 163 | 318 |
| 4.40 | 126.72 | 3.19 | 4.70 | 3.156 | 0.1706 | 4.5706 | 0.1811 | 0.000598 | 0.000553 | 0.001047 | 173 | 491 |
| 4.20 | 119.28 | 3.08 | 4.50 | 3.354 | 0.1925 | 4.3925 | 0.1781 | 0.000705 | 0.000652 | 0.000948 | 188 | 679 |
| 4.00 | 112.00 | 2.96 | 4.25 | 3.572 | 0.2184 | 4.2184 | 0.1741 | 0.000850 | 0.000778 | 0.000822 | 212 | 891 |
| 3.80 | 104.88 | 2.84 | 4.02 | 3.814 | 0.2490 | 4.0490 | 0.1694 | 0.001020 | 0.000935 | 0.000665 | 255 | 1,146 |
| 3.70 | 101.38 | 2.77 | 3.88 | 3.948 | 0.2664 | 3.9664 | 0.0826 | 0.001132 | 0.001076 | 0.000524 | 158 | 1,304 |
| 3.60 | 97.92 | 2.71 | 3.78 | 4.085 | 0.2856 | 3.8856 | 0.0808 | 0.001244 | 0.001188 | 0.000412 | 196 | 1,500 |
| 3.55 | 96.21 | 2.68 | 3.72 | 4.158 | 0.2958 | 3.8458 | 0.0398 | 0.001310 | 0.001277 | 0.000323 | 123 | 1,623 |
| 3.50 | 94.50 | 2.65 | 3.66 | 4.233 | 0.3067 | 3.8067 | 0.0391 | 0.001382 | 0.001346 | 0.000254 | 154 | 1,777 |
| 3.47 | 93.48 | 2.63 | 3.63 | 4.278 | 0.3131 | 3.7831 | 0.0236 | 0.001427 | 0.001405 | 0.000195 | 121 | 1,898 |
| 3.44 | 92.45 | 2.61 | 3.59 | 4.326 | 0.3202 | 3.7602 | 0.0229 | 0.001471 | 0.001449 | 0.000151 | 152 | 2,050 |
| 3.42 | 91.80 | 2.60 | 3.57 | 4.357 | 0.3246 | 3.7446 | 0.0156 | 0.001500 | 0.001486 | 0.000114 | 137 | 2,187 |
| 3.40 | 91.12 | 2.59 | 3.55 | 4.388 | 0.3292 | 3.7292 | 0.0154 | 0.001535 | 0.001518 | 0.000082 | 188 | 2,375 |

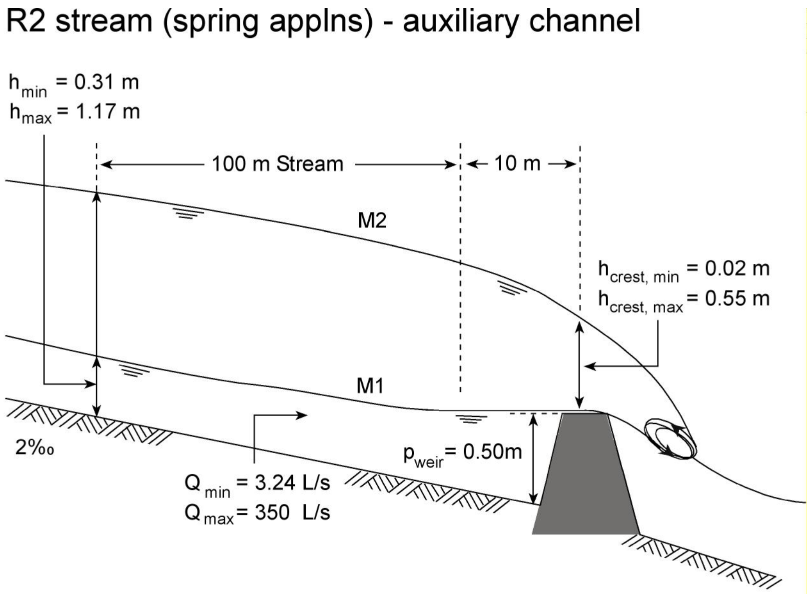
# Appendix 2 Examples of backwater curves in FOCUS ditches and streams




D3 ditch. The two backwater curves (at minimum and maximum discharge) are M1 type curves (Chow, 1959). Flow is subcritical and the water depth at the weir is greater than the normal water depth, which means that as one moves from the weir in the upstream direction, the water depth decreases to the uniform flow depth.

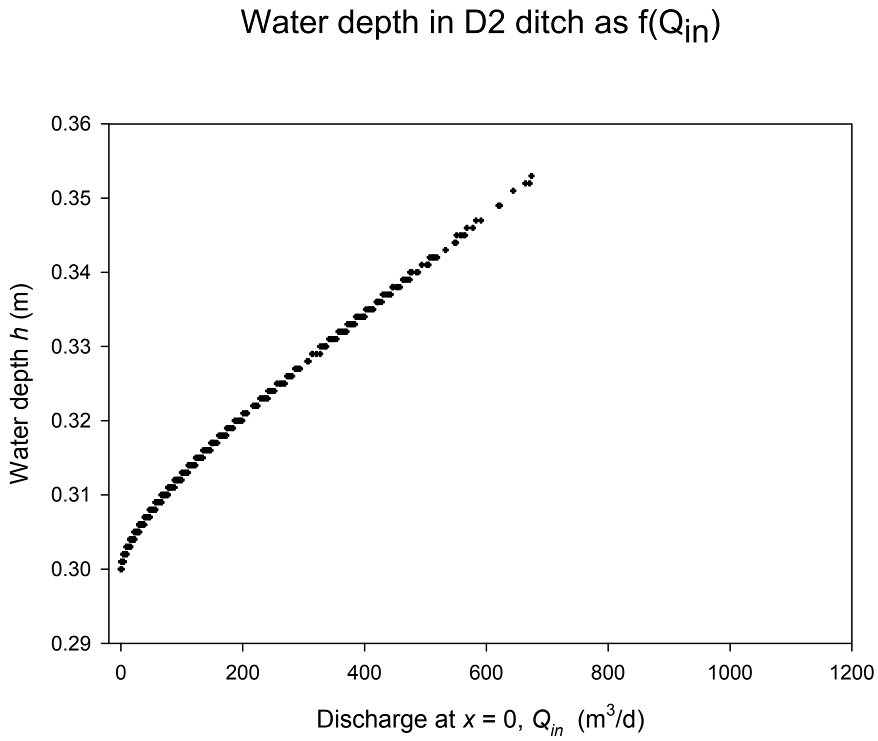



D1 stream. The backwater curve at minimum discharge is an M1 type curve (Chow, 1959). Flow is subcritical and the water depth at the weir is greater than the normal water depth, which means that as one moves from the weir in the upstream direction, the water depth decreases to the uniform flow depth. The backwater curve at maximum discharge is an M2 type curve. Flow is subcritical and the water depth at the weir is smaller than the normal water depth, which means that as one moves from the weir in the upstream direction, the water depth increases to the uniform flow depth.

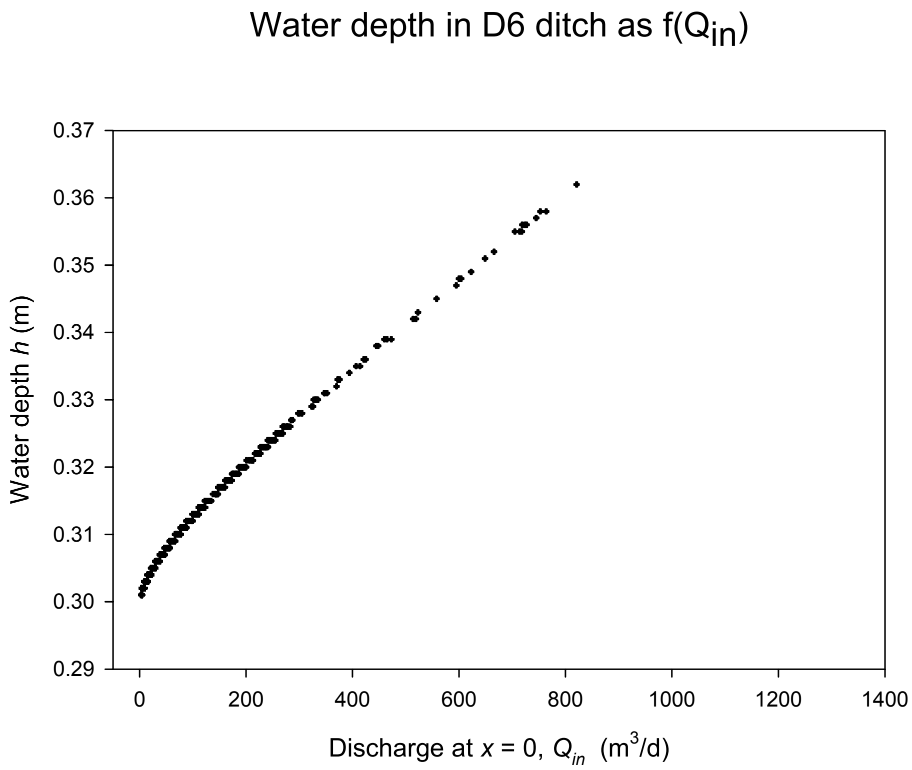


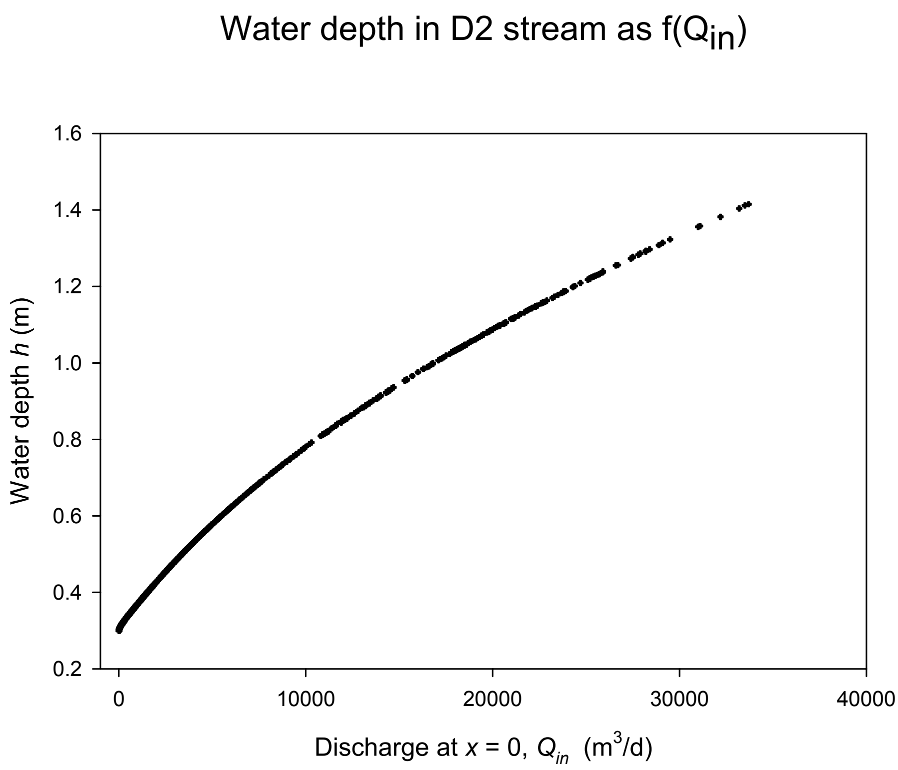

R2 stream (spring applications, so weather year 1 Mar 1977-28 Feb 1978). The backwater curve at minimum discharge is an M1 type curve (Chow, 1959). Flow is subcritical and the water depth at the weir is greater than the normal water depth, which means that as one moves from the weir in the upstream direction, the water depth decreases to the uniform flow depth. The backwater curve at maximum discharge is an M2 type curve. Flow is subcritical and the water depth at the weir is smaller than the normal water depth, which means that as one moves from the weir in the upstream direction, the water depth increases to the uniform flow depth.

# Appendix 3. Water depth *h* as a function of discharge *Q* at *x* = 0 for FOCUS ditches D2 and D6 and FOCUS streams D2 and R4[9]

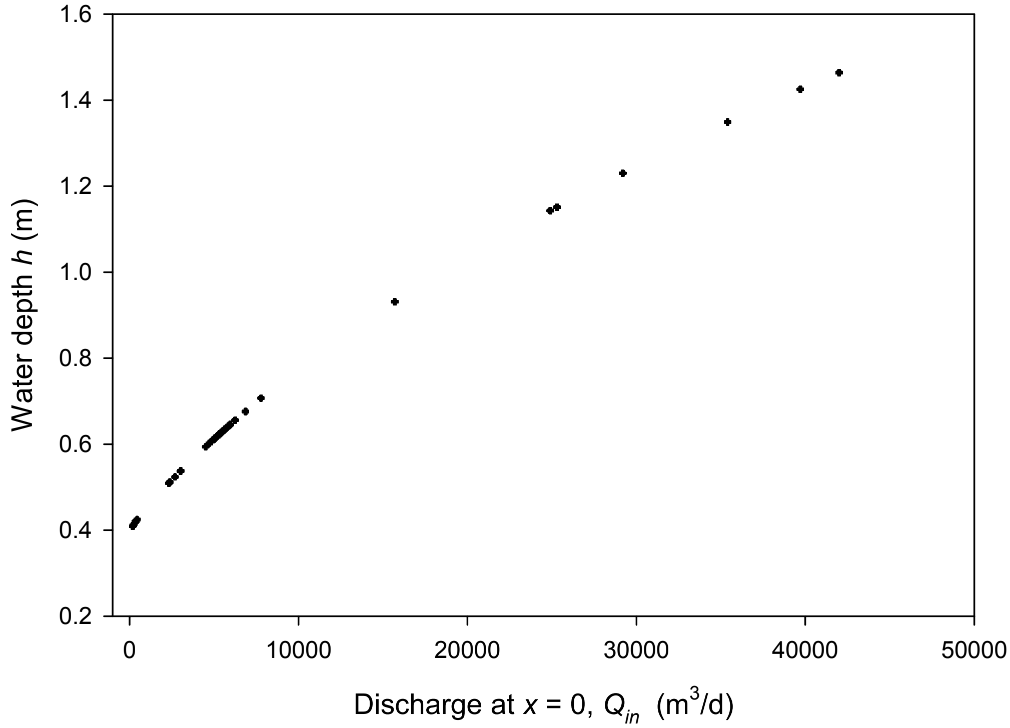



[9] # Graphs based on data of the *.hyb output file of a research version (A6) of FOCUS_TOXSWA_2.2.1, because the *Q-h* pairs of the *.hyb file of the released version 2.2.1 are incompatible; *Q* has been coupled to a water depth *h* of the former calculation time step rather than to the same time step. Note that this error is only 'cosmetic': the mass conservation equations have been solved with correct *Q-h* pairs, so concentrations are not influenced by the error.
# Resolution in iterative water depth calculations was 1 mm, which explains the discontinuous character of notably the D2 and D6 ditch graphs; e.g., 10 distinct steps in water depth are visible between 0.30 and 0.31 cm in the D2 ditch graph.


Water depth in D6 ditch as f($Q_{in}$)
0.37
0.36
0.35
0.34
0.33
0.32
0.31
0.30
0.29
Water depth $h$ (m)
0
200
400
600
800
1000
1200
1400
Discharge at $x$ = 0, $Q_{in}$ ($m^3$/d)


Water depth in D2 stream as f($Q_{in}$)
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
Water depth $h$ (m)
0
10000
20000
30000
40000
Discharge at $x$ = 0, $Q_{in}$ ($m^3$/d)

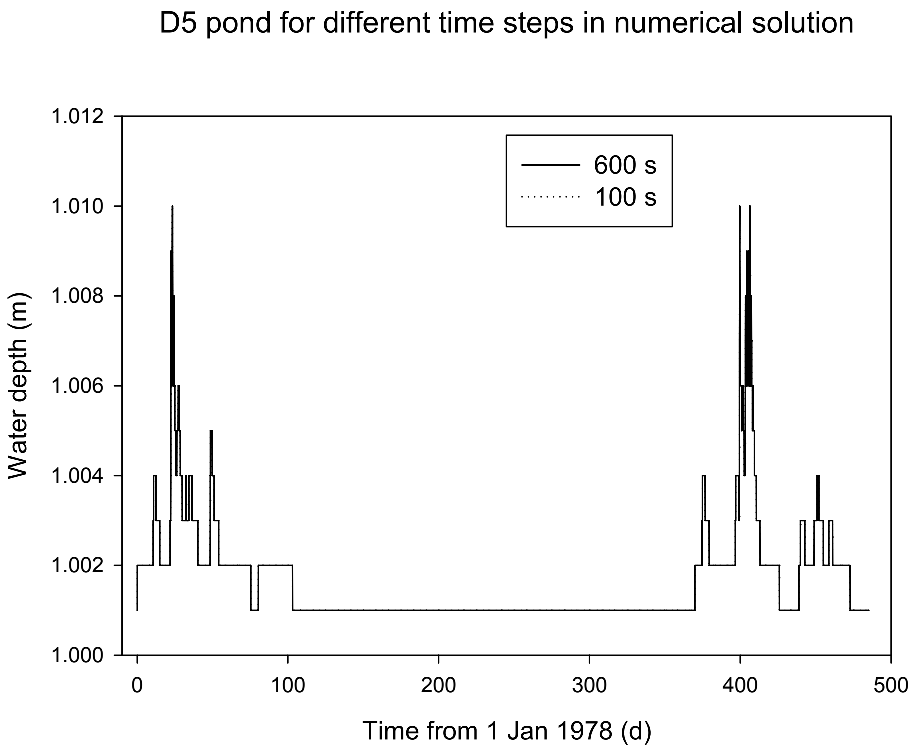
Water depth in R4 stream as f($Q_{in}$) (spring appln)

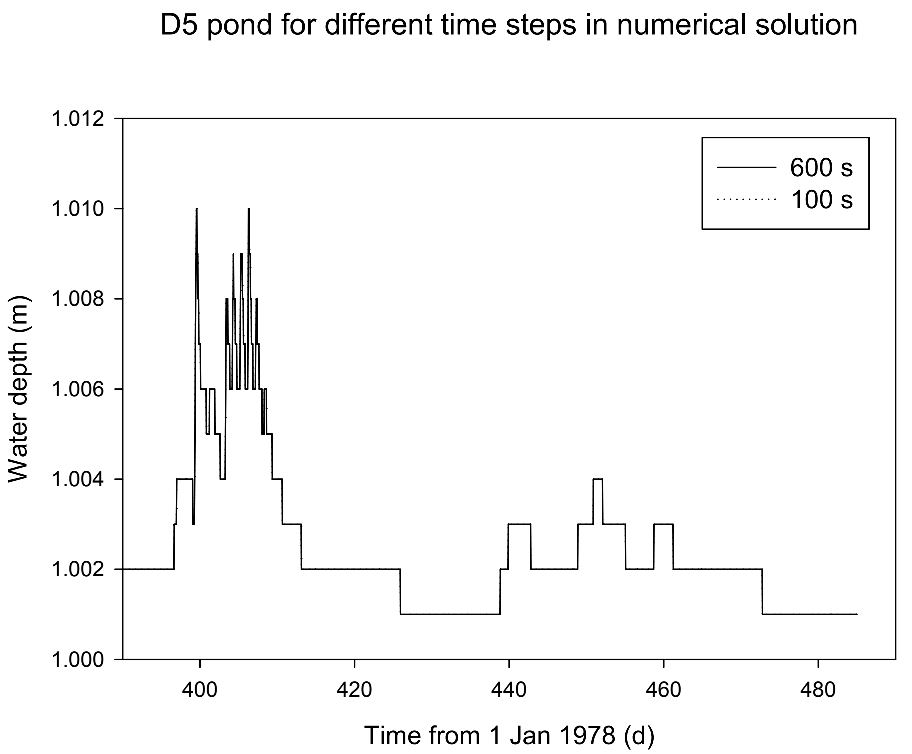


# Appendix 4. Checks on the convergence of the numerical solutions of the water conservation equations for the pond and the watercourse[10]

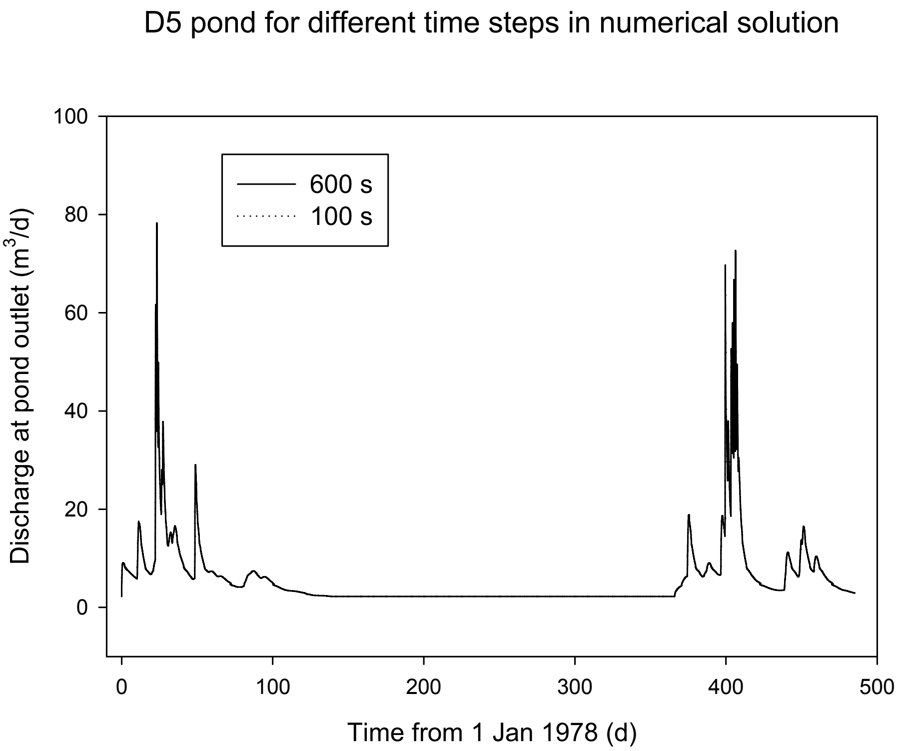
[10] # Graphs of *h(t)* based on data of the *.hyb output file of a research version (A6) of FOCUS_TOXSWA_2.2.1, as mentioned in footnote 9 of Appendix 3.
# The lineic volume flux from drainage or runoff into the watercourse is not affected by the smaller calculation time step of 100 s, because FOCUS_TOXSWA uses hourly values of this term, i.e. no interpolation has been used for this term. All other terms in the water conservation equation have been interpolated, i.e. for steps of 600 s and 100 s, in this test.

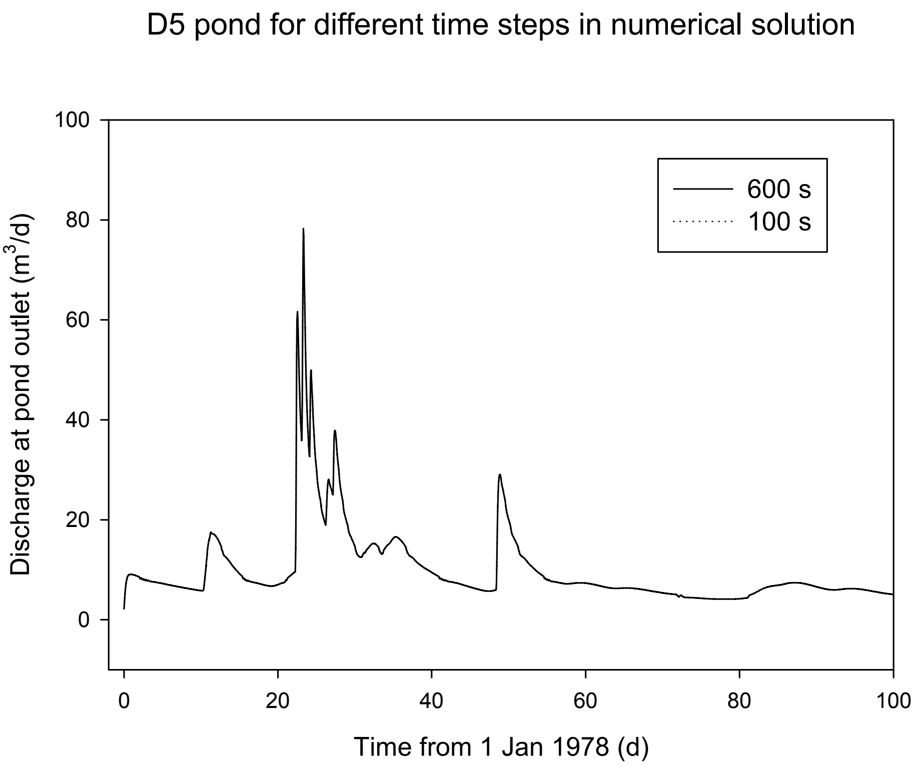
**D5 pond water depth** as a function of time for two different numerical solutions, one with the normal FOCUS calculation time step of 600 s and one with the reduced time step of 100 s. The upper graph shows the entire 16-month simulation period, while the lower graph represents a specific period selected from the upper graph.



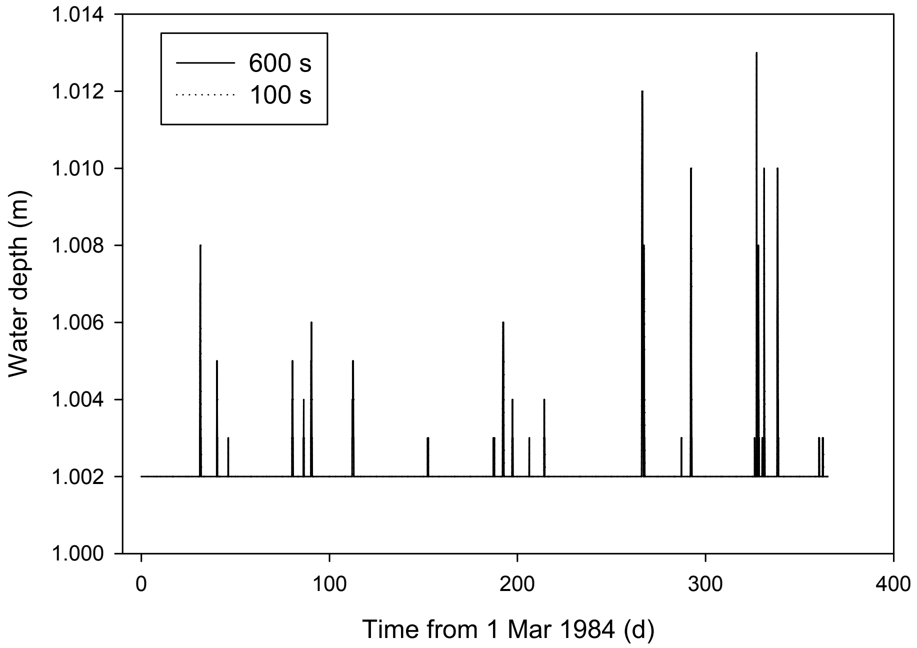
**D5 pond discharge** as a function of time for two different numerical solutions, one with the normal FOCUS calculation time step of 600 s and one with the reduced time step of 100 s. The upper graph shows the entire 16-month simulation period, while the lower graph represents a specific period selected from the upper graph.



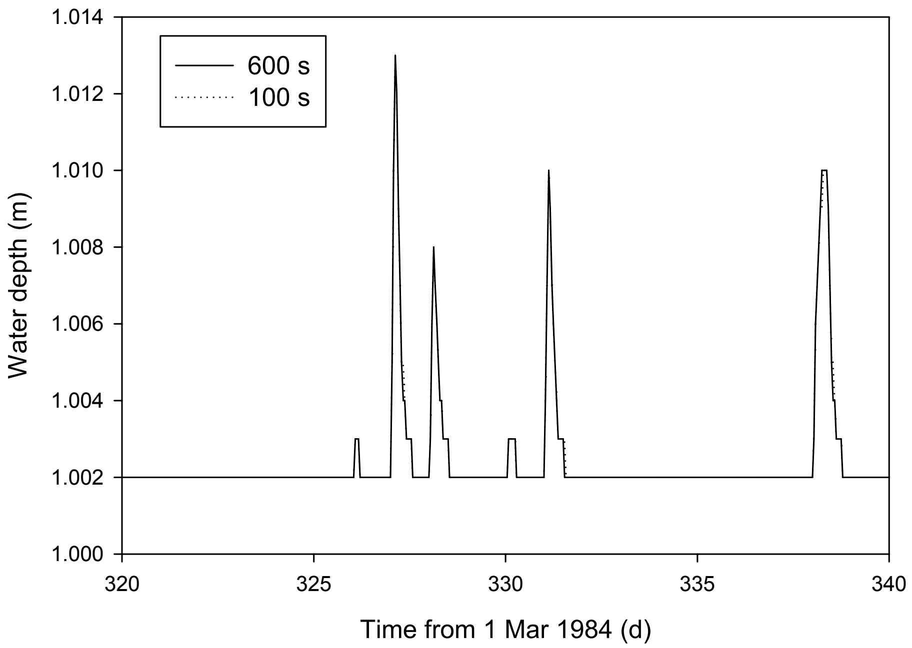



**R1 pond water depth** as a function of time for two different numerical solutions, one with the normal FOCUS calculation time step of 600 s and one with the reduced time step of 100 s. The upper graph shows the entire 12-month simulation period, while the lower graph represents a specific period selected from the upper graph.

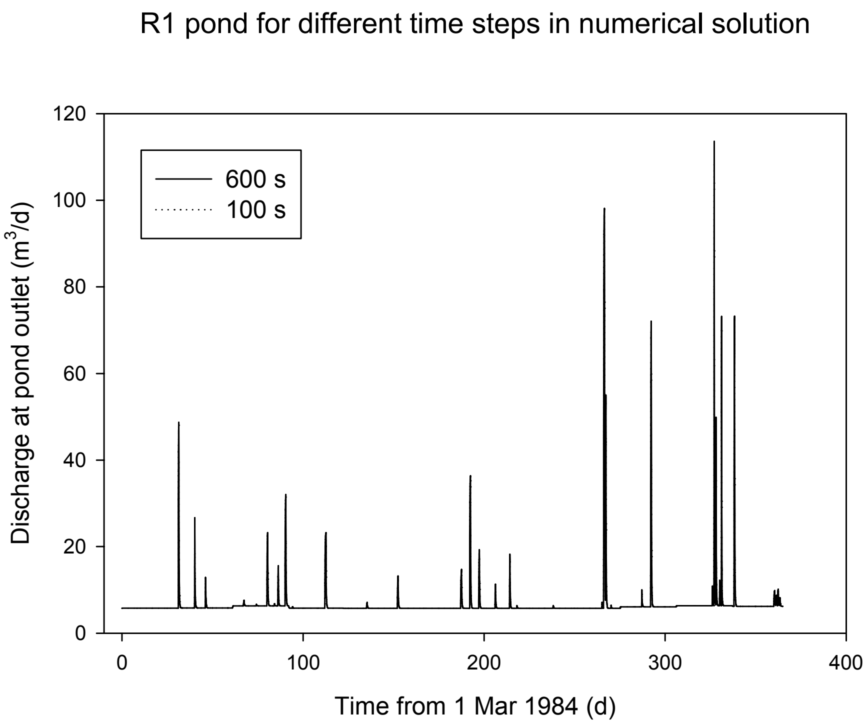
R1 pond for different time steps in numerical solution

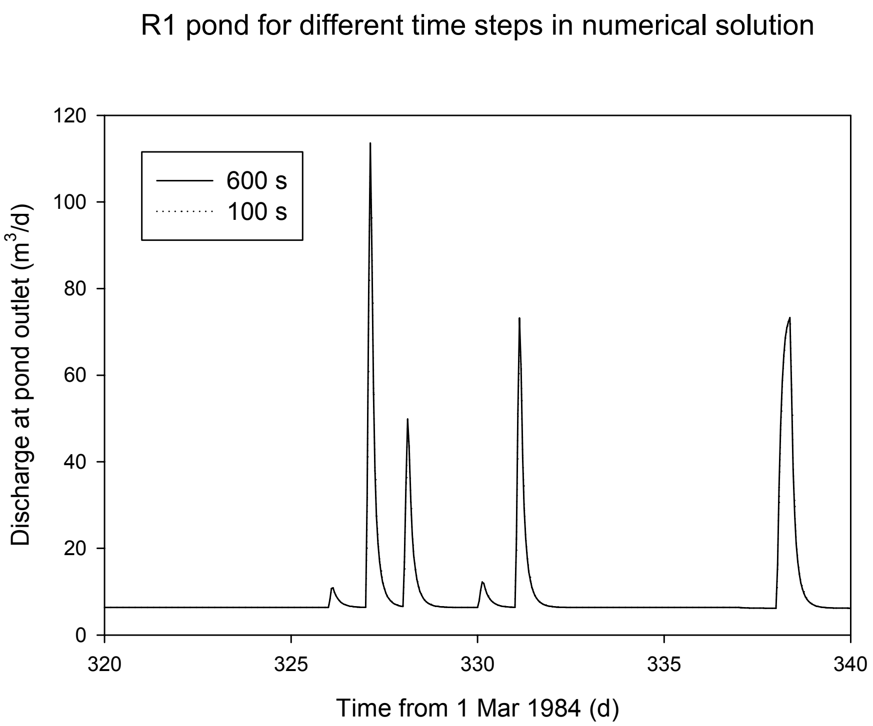



R1 pond for different time steps in numerical solution

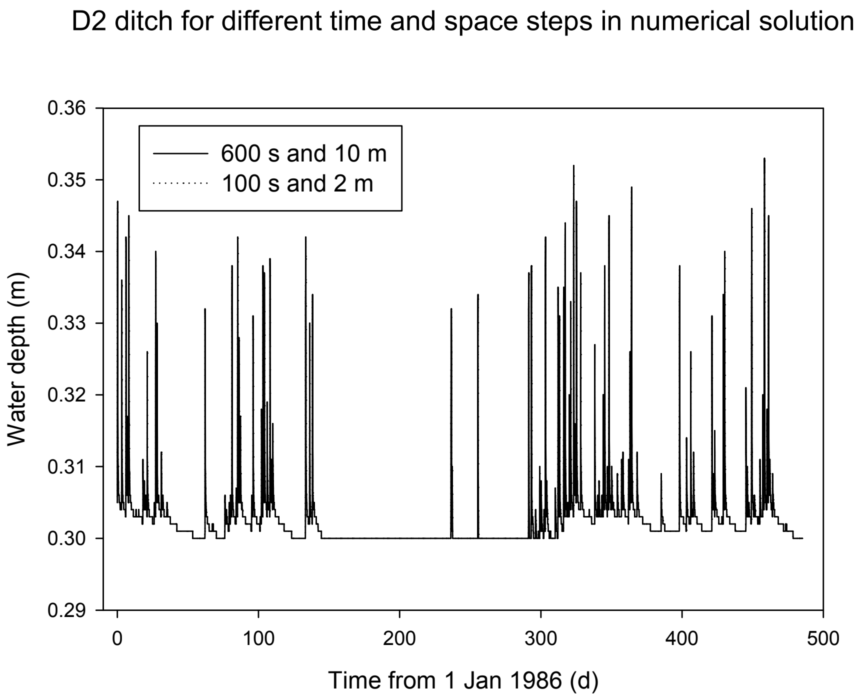


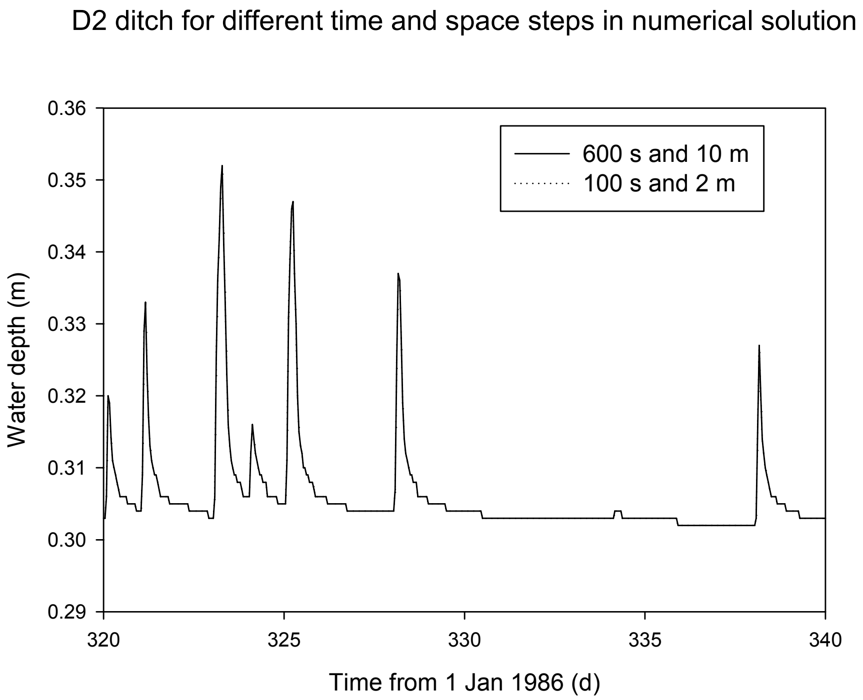
**R1 pond discharge** as a function of time for two different numerical solutions, one with the normal FOCUS calculation time step of 600 s and one with the reduced time step of 100 s. The upper graph shows the entire 12-month simulation period, while the lower graph represents a specific period selected from the upper graph.



**D2 ditch water depth** as a function of time for two different numerical solutions, one with the normal FOCUS time step of 600 s and space step of 10 m and one with reduced calculation steps of 100 s and 2 m. The upper graph shows the entire 16-month simulation period, while the lower graph represents a specific period selected from the upper graph.[11]

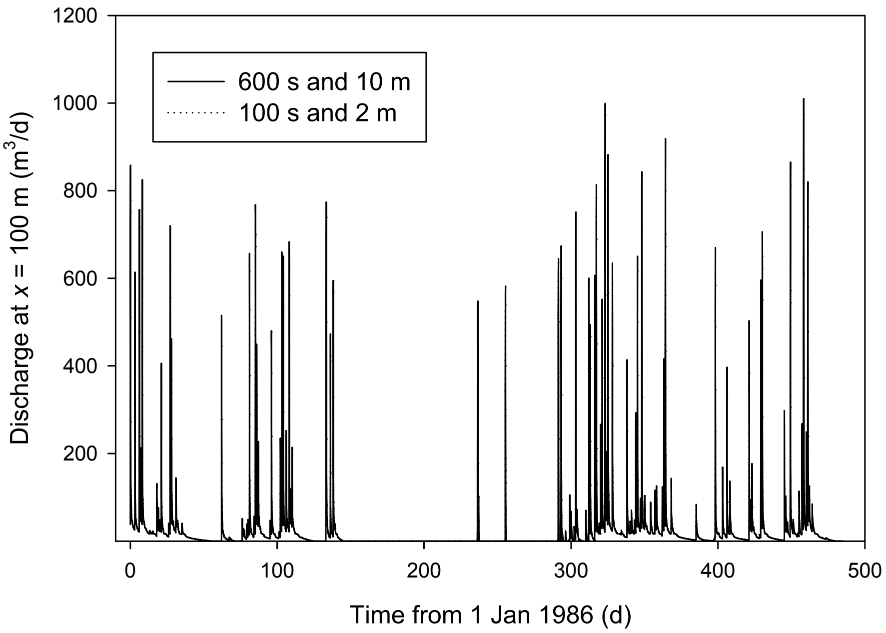


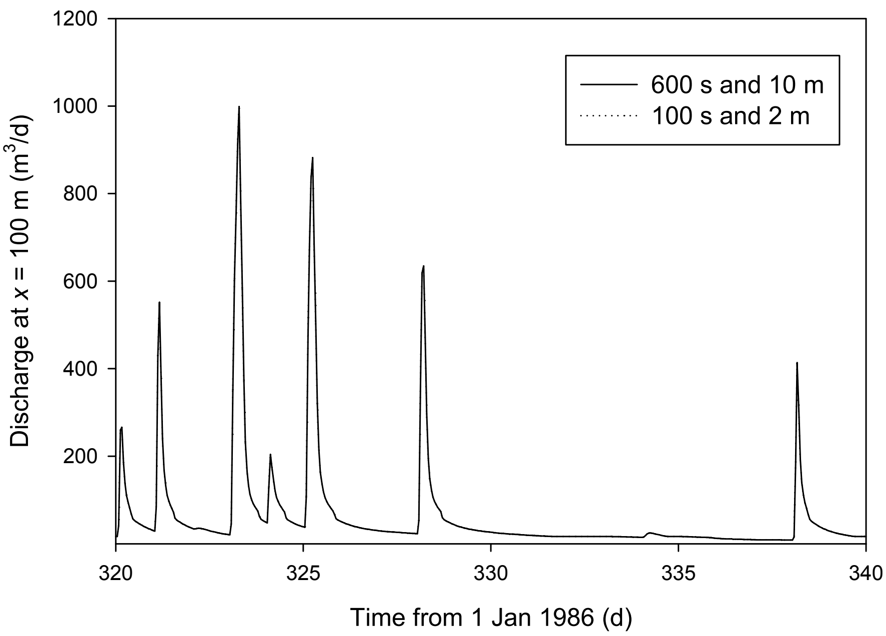

[11] Calculations were done for a base flow of 0.30 $m^3/d$ instead of 0.12 $m^3/d$, which is used in the FOCUS D2 ditch scenario

**D2 ditch discharge** as a function of time for two different numerical solutions, one with the normal FOCUS time step of 600 s and space step of 10 m and one with reduced calculation steps of 100 s and 2 m. The upper graph shows the entire 16-month simulation period, while the lower graph represents a specific period selected from the upper graph.

D2 ditch for different time and space steps in numerical solution

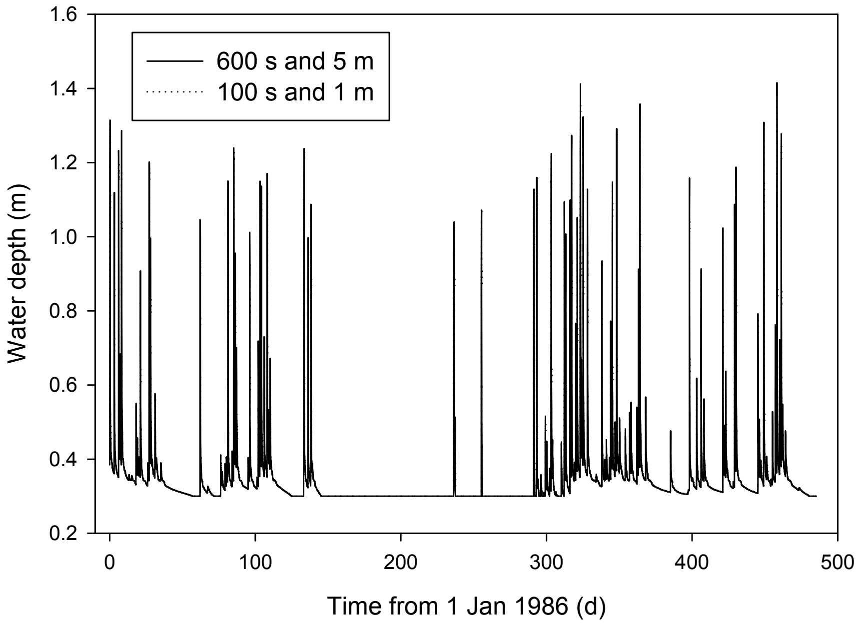



D2 ditch for different time and space steps in numerical solution

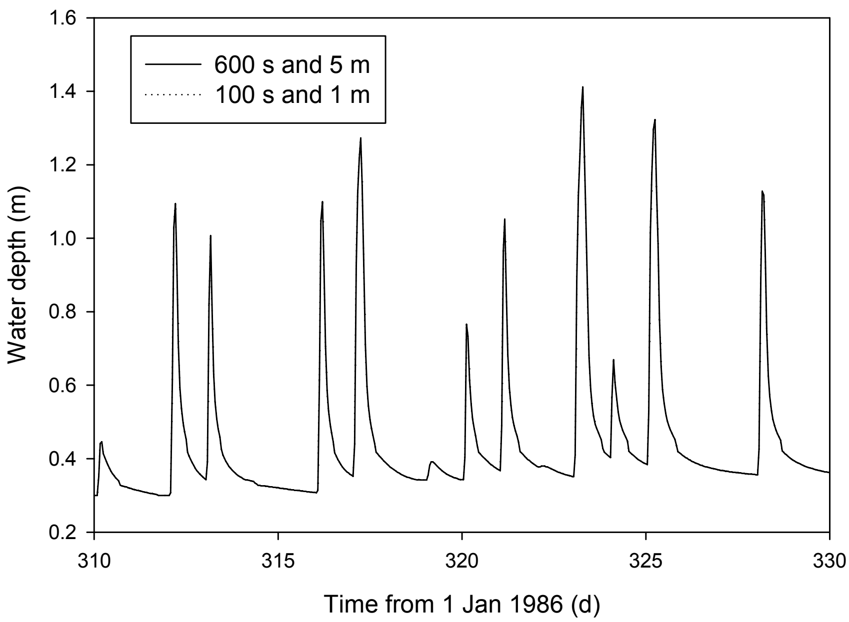


**D2 stream water depth** as a function of time for two different numerical solutions, one with the normal FOCUS time step of 600 s and space step of 5 m and one with reduced calculation steps of 100 s and 1 m. The upper graph shows the entire 16-month simulation period, while the lower graph represents a specific period selected from the upper graph.

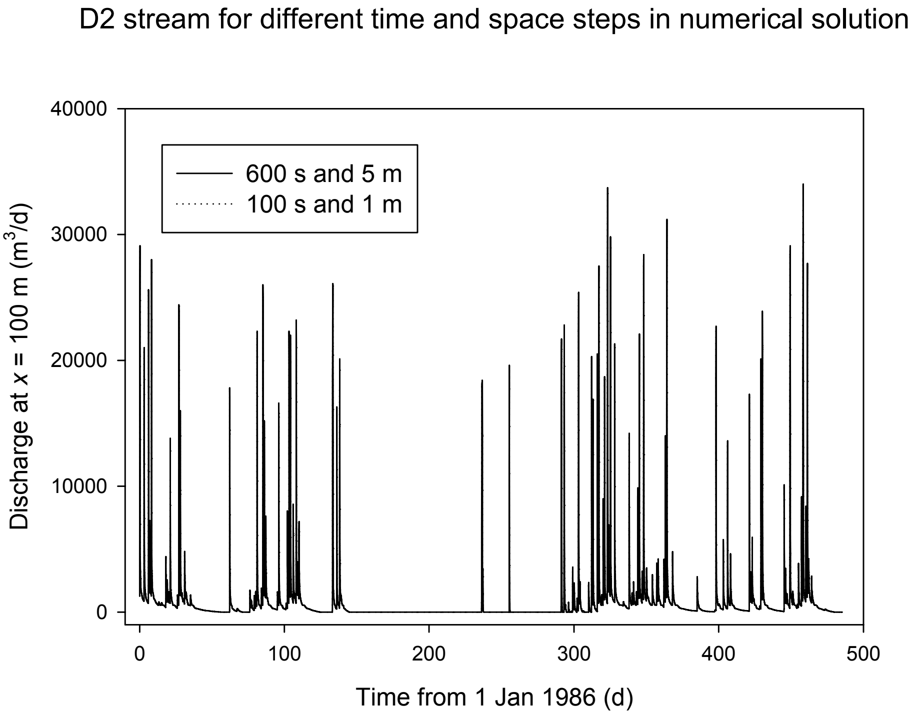
D2 stream for different time and space steps in numerical solution

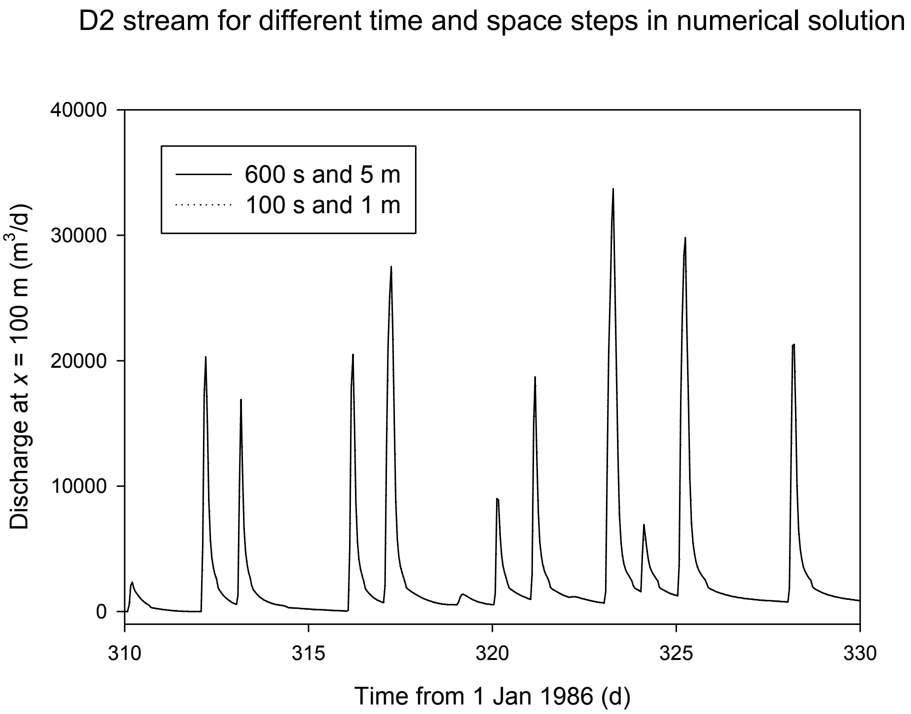



D2 stream for different time and space steps in numerical solution

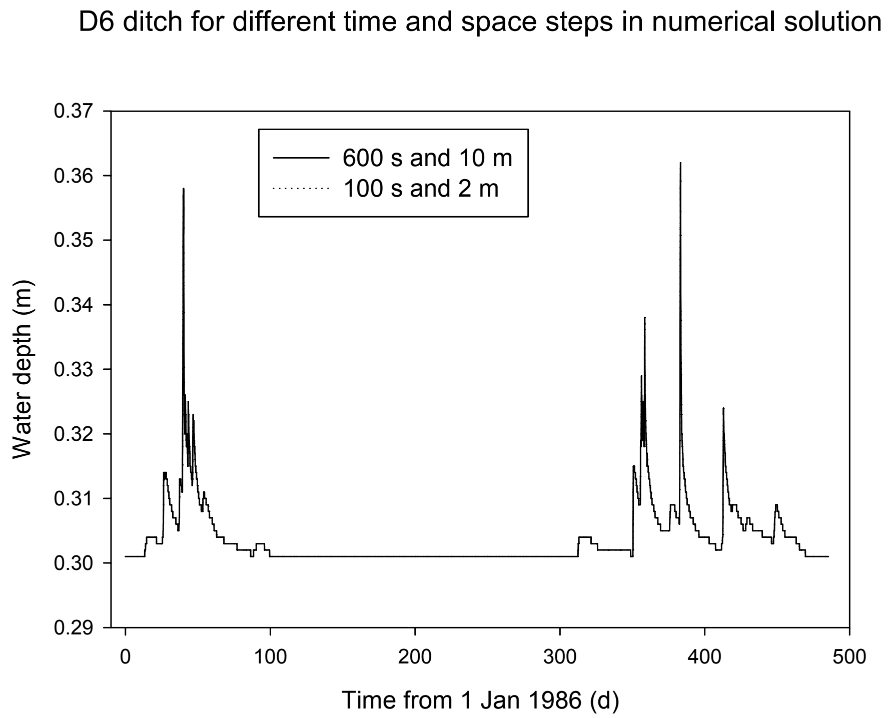


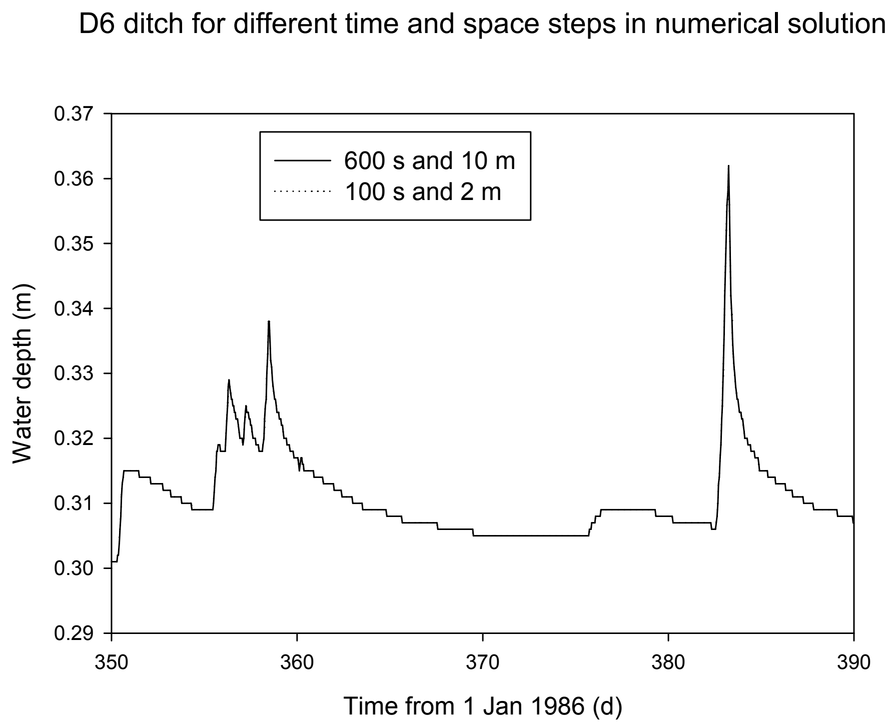
**D2 stream discharge** as a function of time for two different numerical solutions, one with the normal FOCUS time step of 600 s and space step of 5 m and one with reduced calculation steps of 100 s and 1 m. The upper graph shows the entire 16-month simulation period, while the lower graph represents a specific period selected from the upper graph.



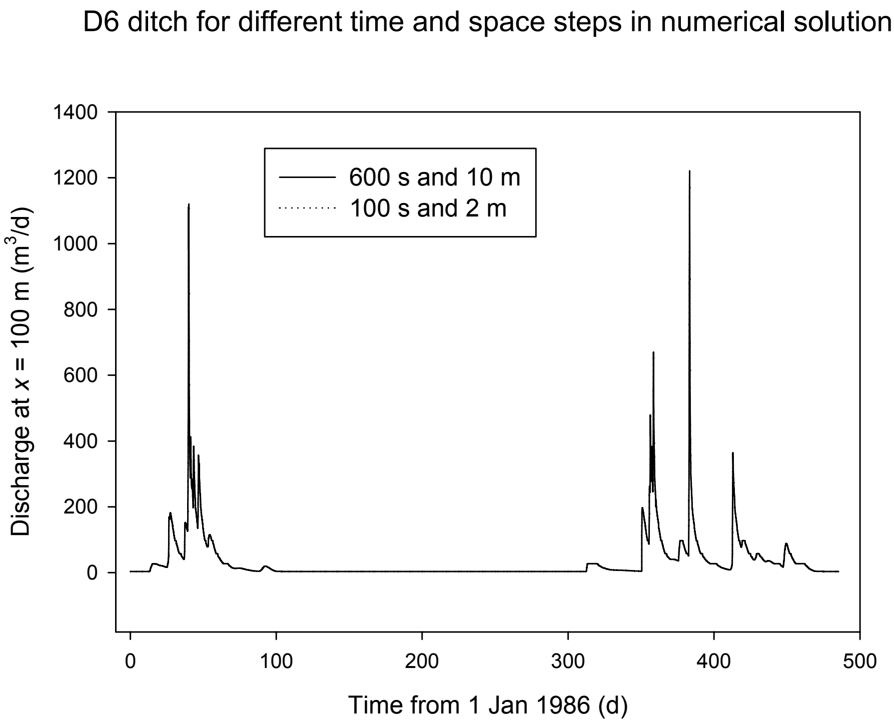



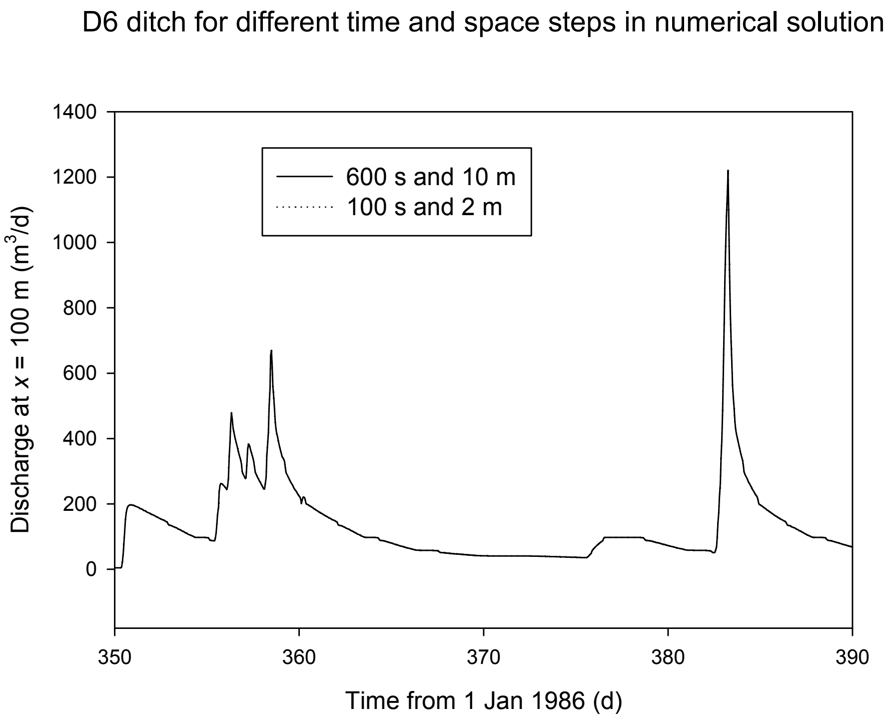
**D6 ditch water depth** as a function of time for two different numerical solutions, one with the normal FOCUS time step of 600 s and space step of 10 m and one with reduced calculation steps of 100 s and 2 m. The upper graph shows the entire 16-month simulation period, while the lower graph represents a specific period selected from the upper graph.



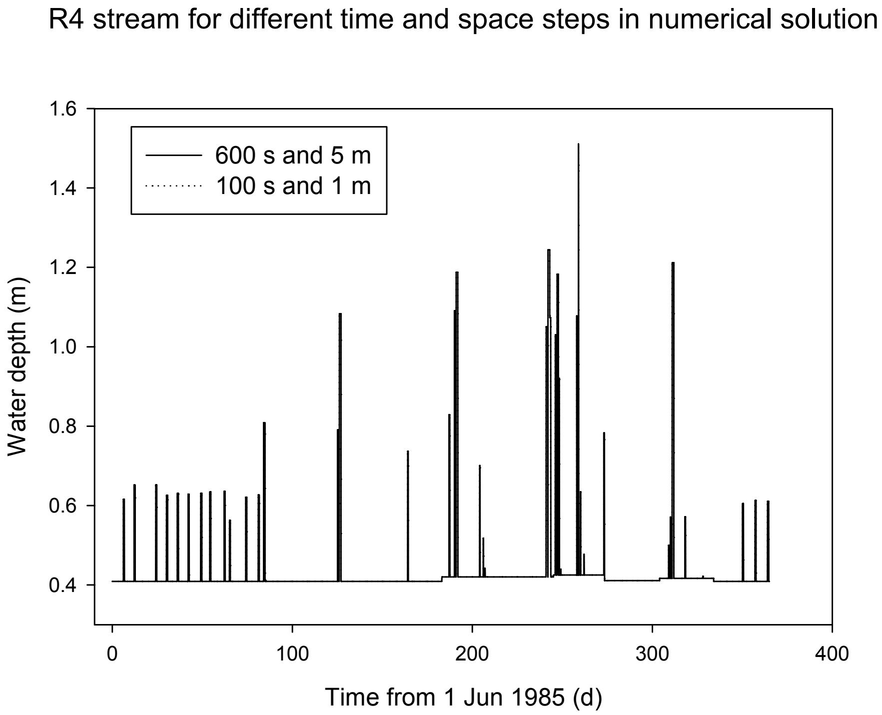



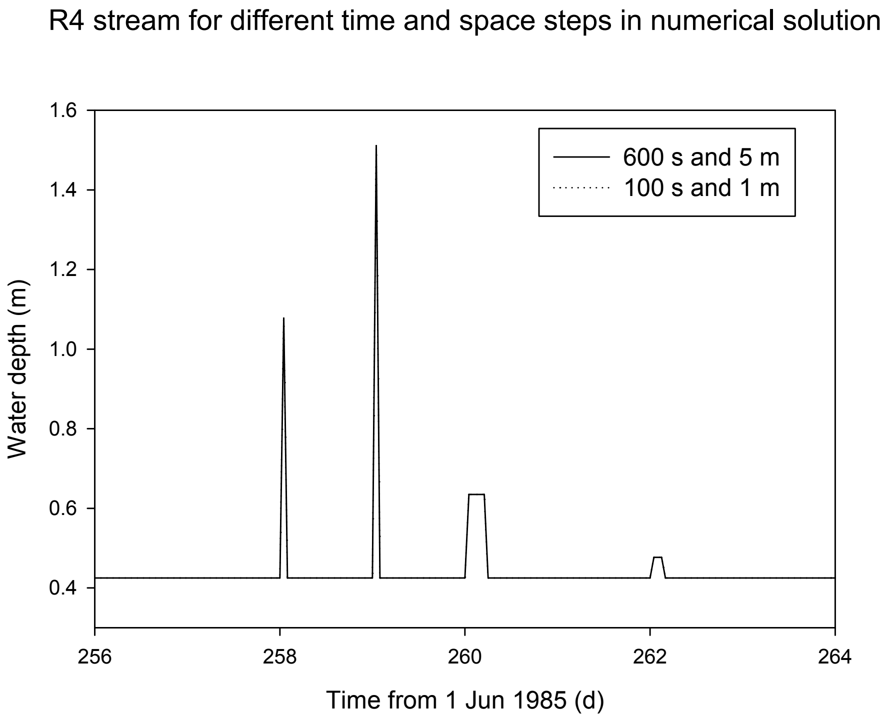
**D6 ditch discharge** as a function of time for two different numerical solutions, one with the normal FOCUS time step of 600 s and space step of 10 m and one with reduced calculation steps of 100 s and 2 m. The upper graph shows the entire 16-month simulation period, while the lower graph represents a specific period selected from the upper graph.



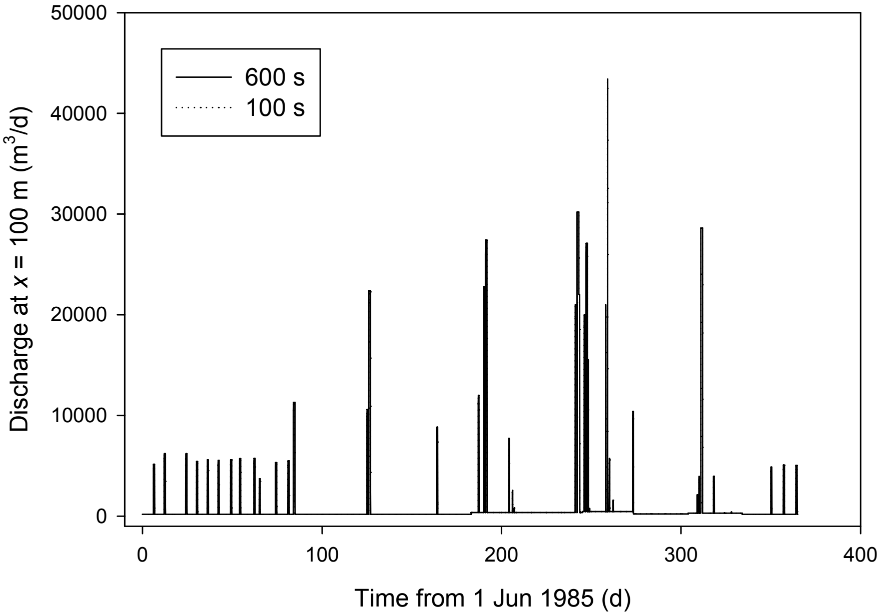
**R4 stream water depth** as a function of time for two different numerical solutions, one with the normal FOCUS time step of 600 s and space step of 5 m and one with reduced calculation steps of 100 s and 1 m. The upper graph shows the entire 12-month simulation period, while the lower graph represents a specific period selected from the upper graph.



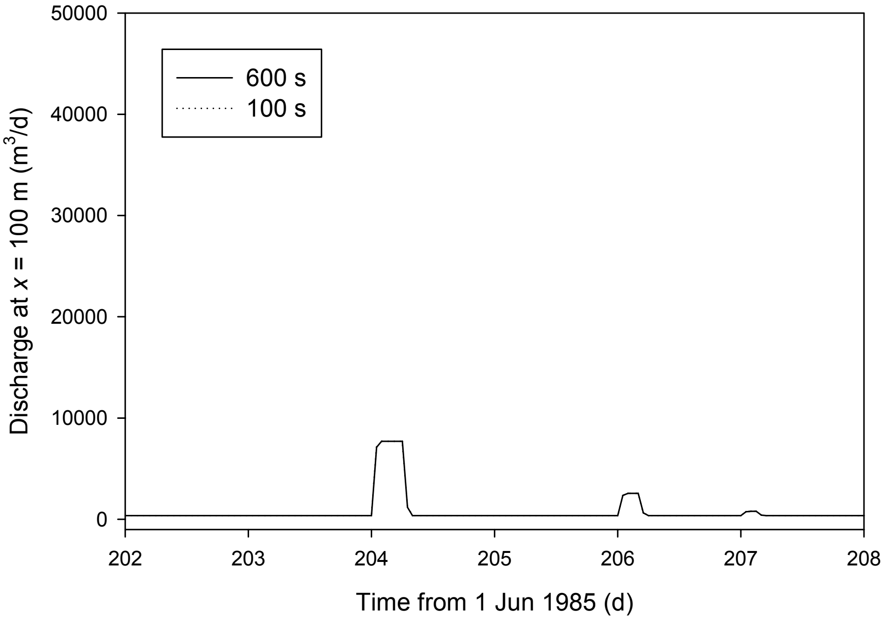



**R4 stream discharge** as a function of time for two different numerical solutions, one with the normal FOCUS time step of 600 s and space step of 5 m and one with reduced calculation steps of 100 s and 1 m. The upper graph shows the entire 12-month simulation period, while the lower graph represents a specific period selected from the upper graph.

R4 stream for different time and space steps in numerical solution

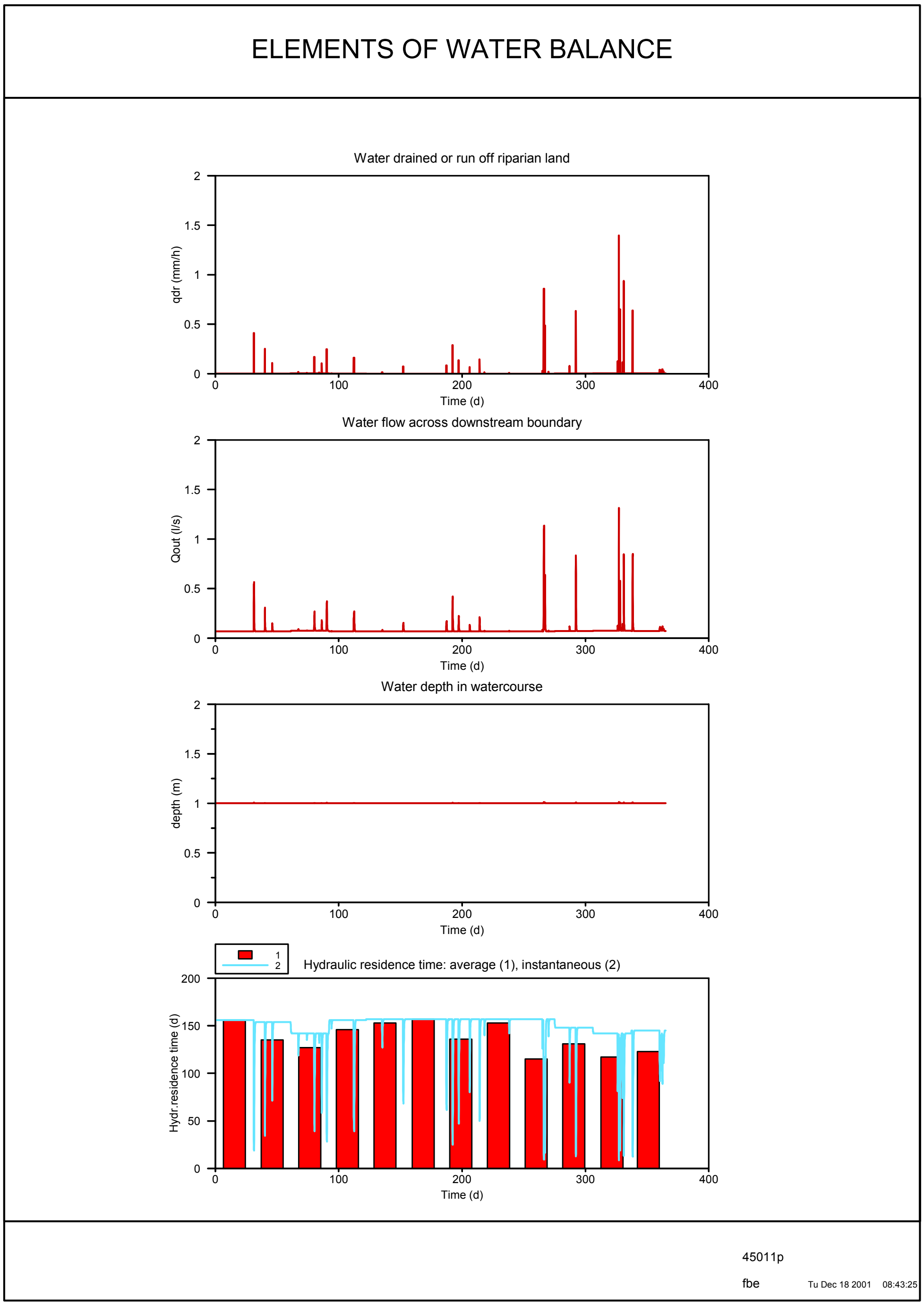



R4 stream for different time and space steps in numerical solution

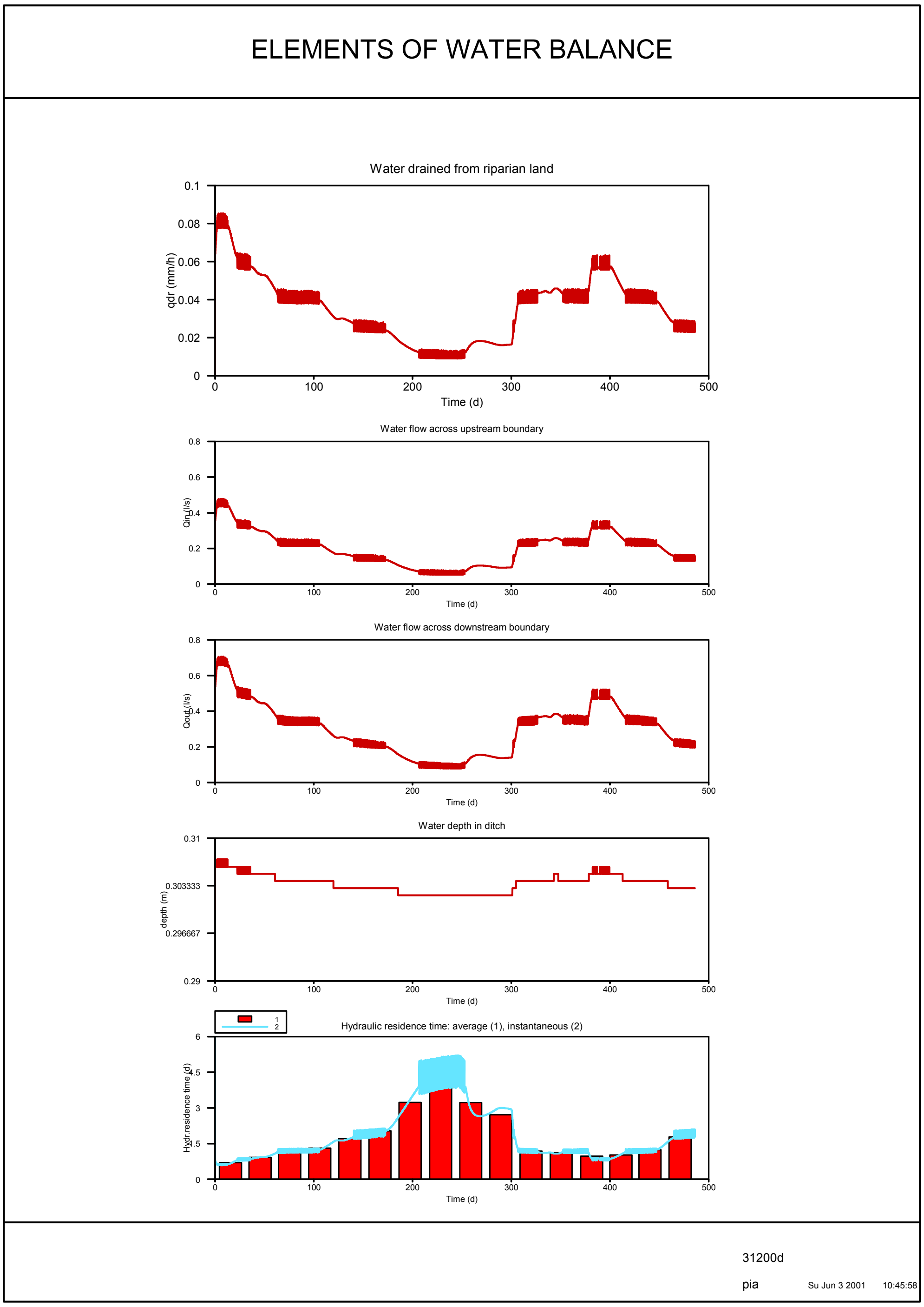


# Appendix 5. Examples of simulated hydrology for FOCUS water bodies

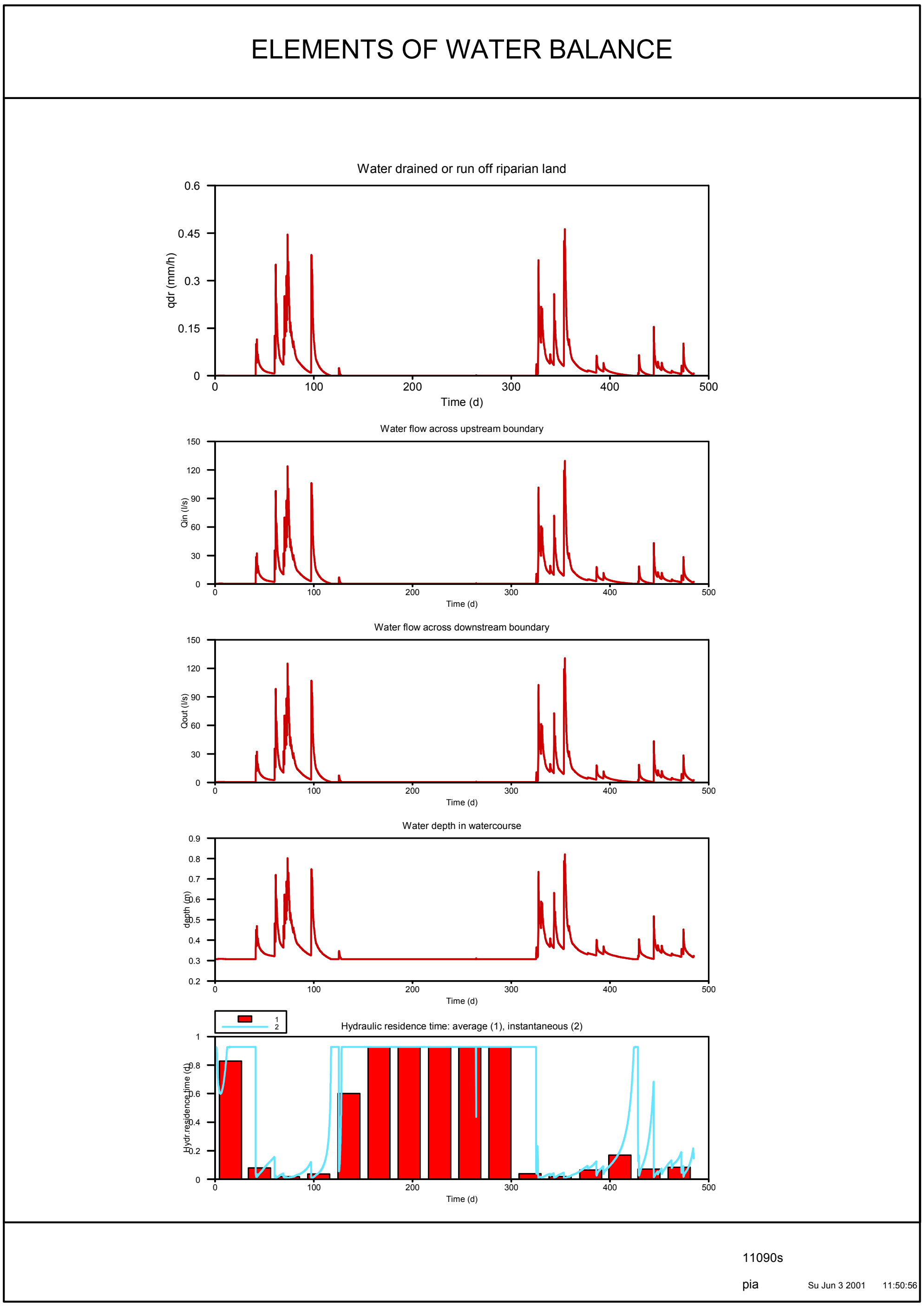
**R1 Pond Hydrology:**
Incoming and outgoing water fluxes, water depth and hydraulic residence times for 1 March 1984 up to 28 February 1985, for an irrigated maize crop with potential pesticide applications from March to May (spring applications)



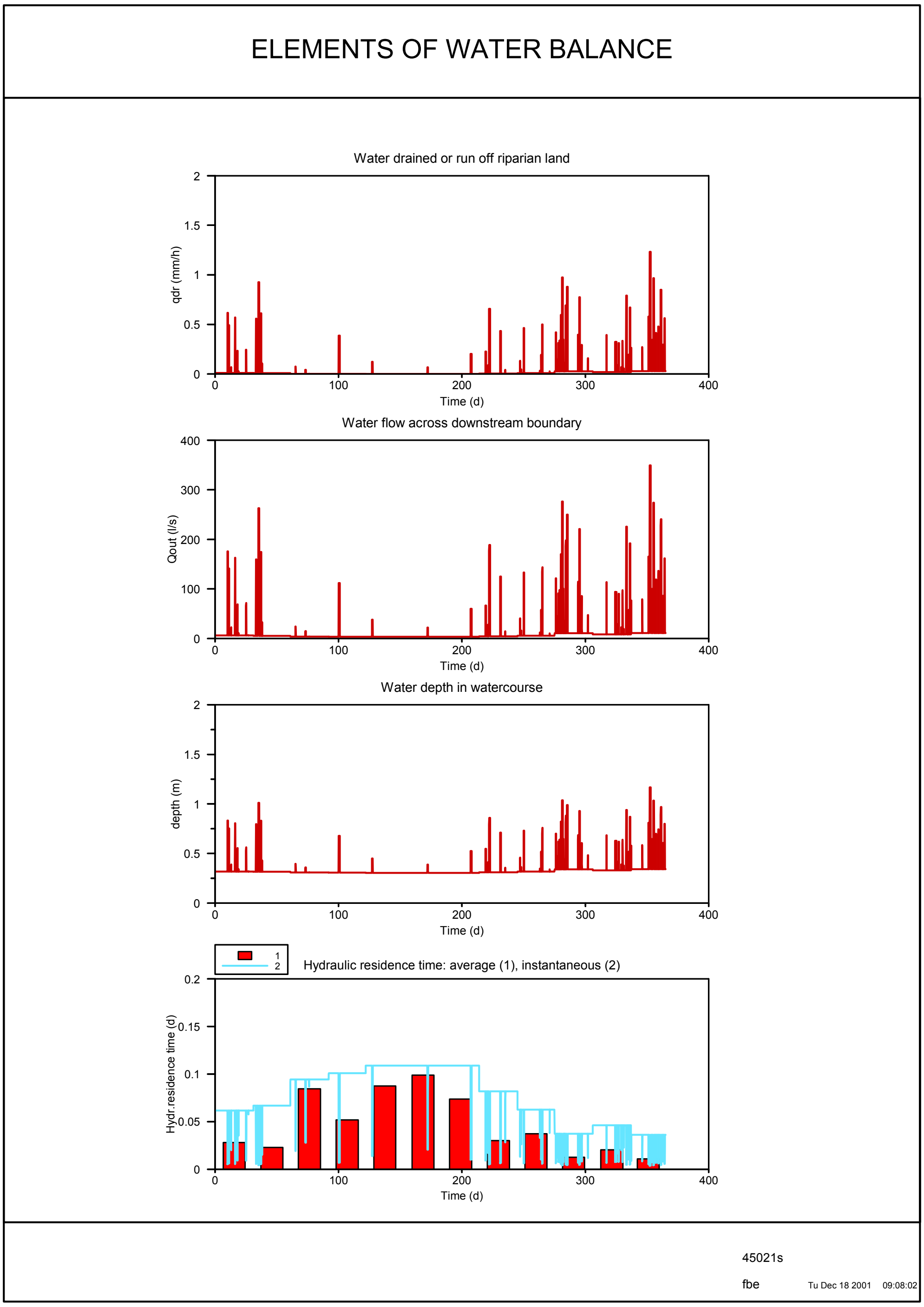
**D3 Ditch Hydrology:**
Incoming and outgoing water fluxes, water depth and hydraulic residence times for 1 January 1992 up to 30 April 1993, for a winter wheat crop



**D1 Stream Hydrology :**
Incoming and outgoing water fluxes, water depth and hydraulic residence times for 1 January 1982 up to 30 April 1983, for a winter wheat crop



**R2 Stream Hydrology:**
Incoming and outgoing water fluxes, water depth and hydraulic residence times for 1 March 1977 up to 28 February 1978, for a maize crop with spring applications



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