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ORIGINAL ARTICLE

Upscaling field scale hydrology and water quality modelling to catchment scale

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Abstract The aim of the research presented in this manuscript is to model the outflow discharge and nutrient load at the outlet of small scale, mainly agricultural catchments. There to two approaches for the simulation of the transport of water and the transport and transformation of nitrogen in the stream were tested and compared. Both approaches use the DRAINMOD and the DRAINMOD-N models to simulate the hydrology and the nitrogen balance of the land phase at the scale of a field/field block/sub-catchment. Both models are used to generate the drain outflow and the nitrate concentration of the drainage water of the field unit considered. The contribution of the field units to the nutrient load of the river are calculated by multiplying the simulated flow weighted N concentrations with drain outflows. In a first approach, called the lumped approach, the water discharge and the nutrient load of field blocks are routed through the river using an exponential model. In this model the nitrate contribution of an individual field block to the nitrate load in the river outlet is calculated assuming first order nutrient decay/attenuation during the transport of the drainage water from the field outlet to the river outlet. The arrival at the outlet section of the nitrate plumes of the field blocks are phased in time based on the velocity profile in the river. The second approach, herein called the complex approach is using the hydraulic river modeling code MIKE 11. This model is using a complex process ADR (advective-dispersive-reactive) equation to calculate the chemical changes in the river water. The comparative analysis between both routing approaches reveals that the lumped approach is able to predict sufficiently accurate nutrient load at the catchment outlet. The complex approach has the advantage of giving a more accurate estimate of the nutrient load at the catchment outlet, resulting in a more precise modeling of the transport and transformation of the nutrient load in streams.

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1. Introduction

During the last decade, an increasing nutrient load has been registered in shallow and deep aquifers, streams and lakes. Previous is mainly due to an over-abundant discharge of nitrogen and phosphorus from both point (municipal sewage, animal feedlots, etc.) and non-point (intensification of farming practices, agricultural runoff and drainage, etc.) sources (El-Sadek *et al.*, 2000). In this study only the effect of nitrogen load from non-point sources on the river quality of small river basins was examined.

A large number of simple to complex water quality models exist for simulating the physical and chemical processes of contaminant transport in streams. Some of the disadvantages of physically based models are dependency on the availability of site-specific parameters; model parameters require additional effort and expense to measure; and physically-based models impose a theory upon the data, a theory that may or may not be complete (Worrall and Burt, 1999). According to Amatya (2000) mechanistic models can describe the processes of constituent transport and transformation on a finer time and space resolution given the availability and accurate estimates of a large number of input parameters. Therefore such models are less likely to be used in day-to-day planning and evaluation. For those circumstances lumped parameter water quality models are often the choice. The objective of this research was to model the drain outflow and nutrient load of field blocks and to route the drain discharge and nitrate load of those blocks or sub-catchments in the river to the basin outlet using two different approaches, a lumped and a physically-based routing model. The lumped routing concept assumes that the decrease in N loads as water travels from the field edge to the basin outlet is exponentially dependent on time in transit and can be described with a single attenuation coefficient. By predicting the travel times from each field to the outlet on a continuous basis, this approach to nitrogen modeling can be applied on either a distributed (field by field) or aggregated (field block or sub-catchment) basis, in both space and time. In the complex approach, the MIKE 11 model (DHI, 1998) is used to route the nutrient load from the sub-catchments to the concentration of the river water at the basin outlet. For reconstructing the transfer of nitrogen from the soil-crop system of a field/field block/sub-catchment to the river use was made of the quasi two-dimensional mechanistic flow model, DRAINMOD (Skaggs, 1981), in combination with DRAINMOD-N (Brevé *et al.*, 1997).

The DRAINMOD/DRAINMOD-N/GIS/exponential decay model and the DRAINMOD/-DRAINMOD-N/GIS/MIKE 11 approaches were tested using time series of observed nitrate loads at the outlet of the Molenbeek river basin (57.44 km^2). The study was carried out to determine in a rural catchment the contribution from organic and inorganic nitrogen fertilizers to the nitrate load found in the surface water. The DRAINMOD and DRAINMOD-N models allow calculating at the scale of an individual field or field block the daily nitrate leaching for a given soil, crop, climate, geo-hydrological and farming condition. The used water and nitrogen model covers the entire land phase of the hydrological cycle from the source on the soil surface, through the soil profile and the shallow drainage system. The GIS pre-processes the river basin data in field specific data in a format suitable for the simulation models, and summarizes the main simulation results in tables and maps. The time series of the nitrogen load at sub-catchment level is used as input in the lumped (exponential decay-time rating model) and the physically based (MIKE 11) approaches. The model results of both routing approaches were tested versus the NO_3-N load in the river water measured at the basin outlet.

Table 1 The MAP fertilizer standards (as published in 1995)

Crops	Nitrogen (kg ha^{-1})		
	Animal or organic	Chemical or mineral	Total amount
Pasture	150	200	350
Maize	125	150	275
Crops with low nitrogen need	55	70	125
Other crops e.g.: potato, beets, winter wheat	125	150	275

2. Study area

The two routing approaches were implemented and evaluated for the Molenbeek catchment, a tributary of the Dender basin. The river Dender basin is located to the west of Brussels in a region with a rolling landscape. It is a tributary of the river Scheldt and has its springs in the Walloon region. Because of the rolling topography in the source area and the relative small water holding capacity of the soils, the flow in the tributaries of the Molenbeek are characterized by relative large discharge fluctuations. The base flow discharges are small, while the response to rainfall is large. The Molenbeek catchment has a total area of 57.44 km^2 (Willems, 2000). It is a narrow and relatively strong indented catchment. The upstream part is rural, while the downstream part is more urbanized (village of Mere, Erpe and Hofstade). One limnigraphic station (hourly water level data and rating curve) is available at Mere (station 20) (Radwan *et al.*, 2000, 2001). The average monthly rainfall and evapotranspiration in the catchment for 30-year data are 68.7 and 34.8 mm, respectively. A dominant flat to slightly undulating topography and a shallow water table characterizes the catchment. Large areas of the catchment are artificially drained. Since the exact fertilizer package per field for the period of analysis could not be reconstructed the threshold values for N-fertilizers, as specified in the fertilization standards of the Flemish Government were applied. The nitrogen standards according to the Manure Action Plan (MAP, 1995) are listed in Table 1. Those standards were taken as the fertilizer practice for each field block/sub-catchment in which the catchment was divided. The foregoing might have led to an underestimation, respectively to an overestimation, of the nitrate leaching from the sub-catchments. Figure 1 shows the relation between flow and nitrate-nitrogen concentration in the catchment.

For the application of the simulation models, DRAINMOD and DRAINMOD-N, the following information was collected for each of the sub-catchments: climate, land use, soil type, water and nitrogen status of the soil profile at the start of the simulation period, and nitrogen fertilizer practice. The model input was approximated for all fields within each sub-catchment. Soil information was derived from the digitized soil map. Based on the soil series observed in the region, statistical profiles were selected from the soil information system AARDEWERK-BIS (Van Orshoven *et al.*, 1991). The core soil series of the legend of the Belgian soil classification system is built of a three letter combination representing texture of the topsoil, natural drainage class and soil profile development. The series is further specified by qualifiers, which refer to substratum, type of parent material and soil phase (Van Orshoven, 1993). The first letter in the three letter soil code refers to the soil texture, e.g. Z, which stands for a coarse textured cover sand and sand dunes, and is named after the mineral composition of the top 30 cm of the soil profile. Changes in texture with depth due to the presence of a substratum, are given by an alphanumeric symbol in front of the texture symbol in the soil code. The substratum is specified in case it occurs at shallower depth than 80 cm, e.g., sLba. If it occurs between 80–120 cm it is given as a (x)Lba (Van Orshoven,

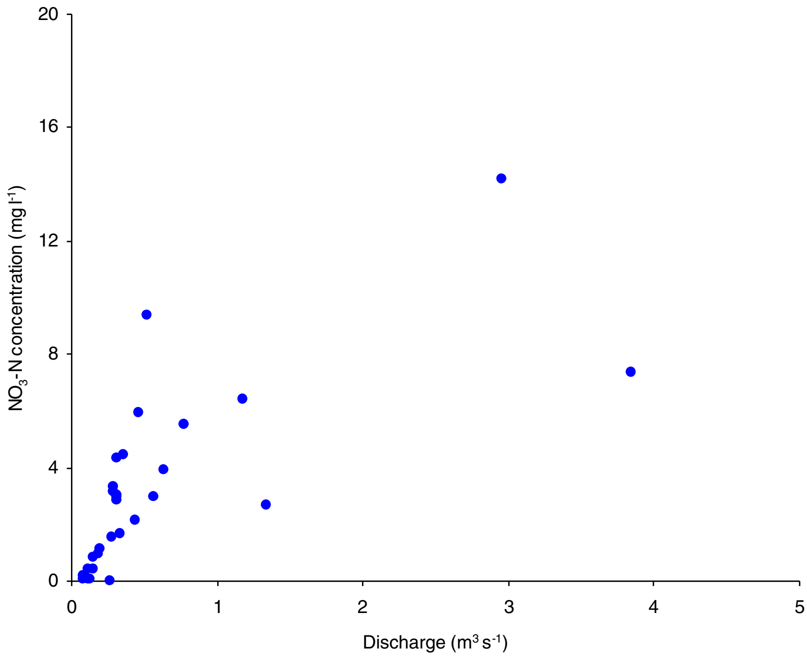

Fig. 1 The relation between flow and nitrate-nitrogen concentration at the catchment outlet

1993; Feyen *et al.*, 2000; Vázquez *et al.*, 2002). The drainage class is determined on the basis of depth to gley phenomena in the soil profile. The third letter in the soil code stands for the profile development. Four different soil types can characterize the soil distribution in the Molenbeek basin. The soil types are primarily silt loam soils (Lca, Ldc, Aba and Ada). The soils have different drainage conditions ranging from dry (a) to medium wet (e), and profile development ranging from poorly (p) to strongly differentiated horizons (g). For the soil profiles the geometry of the profile (boundaries of the pedogenetic horizons), the soil hydraulic parameters and the soil organic carbon content were derived from the soil information system. Land use in the catchment is mainly pasture and arable land. The latter was derived using the TELSAT land use map (1995) of Flanders (OC GIS, Vlaanderen) providing information on land use for grid cells 30×30 m. It provides information on the spatial distribution of land use types. Making abstraction of the smaller agricultural land units the main four agricultural uses in the catchment are pasture, maize, fodder beet and potato (Vanongeval *et al.*, 1996). The percentages of the land use areas in the Molenbeek catchment are listed in Table 2. The land use conditions for the simulation periods were assumed constant.

3. Routing models

3.1. Exponential decay based lumped parameter model

The drain discharge rate and the flow-weighted concentration of the drainage water vary from year to year due to change in weather conditions (Amatya, 2000). Their value should

Table 2 The main land use classes in the Molenbeek catchment

Code number	Land use	% of area
2	Discontinuous urban fabric	23.13
3	Industrial or commercial units	0.92
12	Potato	24.96
18	Pasture	10.36
20	Fodder beet	30.14
21	Maize	10.48

be known if one wants to simulate the transport of water and nitrogen and the transformation of the latter in the river. In the absence of measured data they can be simulated using DRAINMOD and DRAINMOD-N. In this study it was assumed that there are no sources or sinks of the constituent other than the natural decay, commonly described by first order kinetics, in contrast to the transformation kinetics in big streams and rivers near the mouth of estuaries. The exponential decay method is based on a gross assumption that dispersion of the constituent concentration along the rivers and ditches is totally negligible due to minimal effects of tidal influence and there are no sources or sinks of the constituent, other than the natural decay (Loucks *et al.*, 1981). The method as developed by Loucks *et al.* (1981) is used to calculate the total nitrate load at the catchment outlet. Mathematically, the cumulative annual load (L) of the nutrient at the catchment outlet can be defined as (Amatya, 2000):

$$L = \sum (L_i) \tag{1}$$

where,

$$L_i = L^*_{io} DR \tag{2}$$

$$\text{Delivery Ratio, } DR = \exp(-K^* T_i) \tag{3}$$

and L_i is the ultimate annual nutrient load (after attenuation) delivered from a field (i) to the catchment outlet due to an initial field loading L_{io} at that field edge; K is the nutrient decay/attenuation rate during its transport and T_i is the travel time of nutrient for its transport from the field edge (i) in the stream network to the catchment outlet;

$$\text{Initial Field Loading, } L_{io} = \text{Nitrate load}^* \text{Area}; \tag{4}$$

The value of the nitrate load is based on a given land management practice (soil, crop/vegetation, and water management). It can be obtained from simulations using DRAINMOD-N for a field of interest. General values on loading can be estimated as a product of annual outflow measured or simulated using DRAINMOD and nitrate concentration, e.g. annual average nutrient concentration, obtained by direct measurements or DRAINMOD-N simulations. The values of nutrient decay or attenuation rate (k) may vary with both the season and location in the river, with generally higher values during low flows and vice versa. The travel time [T] is calculated as:

$$T_i = \text{Distance/Velocity} \tag{5}$$

where distance is the length of the nutrient travel path specified along the canal/stream from the field edge to the outlet [L]. Distance is measured along the specified flow path passing through the nodes of the canal/stream network that is identified and defined during the delineation of the individual fields with its specified outlet in the canal/stream network, and velocity is the average velocity of nutrient movement along the canal [L T^{-1}] and is a function of season or event and location in the catchment.

3.2. MIKE 11 model

The MIKE 11 model consists of different modules of which in this study were used the hydrologic (NAM), hydrodynamic (HD) and water quality (WQ) modules. The MIKE 11 hydrodynamic module uses an implicit, finite difference scheme for the computation of the flow in the rivers. The module can describe sub-critical as well as super-critical flow conditions through a numerical scheme that adapts in time and space according to the local flow conditions. Advanced computational modules are included for the description of flow over hydraulic structures, including possibilities to describe structure operation. The formulations can be applied to looped networks and quasi-two-dimensional flow simulation on flood plains. The water quality module in MIKE 11 was developed by the VKI (Water Quality Institute, Denmark). It describes the basic processes of river water quality in areas influenced by human activities, e.g. oxygen depletion and ammonia levels as a result of organic matter loads. The WQ module solves the system of coupled differential equations describing the physical, chemical and biological interactions in the river.

Concentrations of nitrate are calculated in MIKE 11 by taking into consideration advection, dispersion and the most important biological, chemical and physical processes. The one-dimensional (vertical and lateral variation integrated) equation for the conservation of mass of a substance in solution, i.e., the one-dimensional advection-dispersion equation, reads as follows:

$$\frac{\partial AC}{\partial t} + \frac{\partial QC}{\partial x} - \frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right) = -AKC + C_2 \cdot q \tag{6}$$

where C is the concentration (arbitrary unit), D is the dispersion coefficient [$L^2\,T^{-1}$], A is the cross-sectional area [L^2], K is the linear decay coefficient [T^{-1}], C_2 is the source/sink concentration [$M\,L^{-3}$], q is the lateral inflow [$L^2\,T^{-1}$], x is the space co-ordinate [L] and t is the time co-ordinate [T]. The equation reflects two transport mechanisms: advective (or convective) transport with the mean flow and dispersive transport due to concentration gradients. The main assumptions underlying the advection-dispersion equation are that the chemical component is instantaneously mixed over the cross-sections, and the substance is conservative or subject to a first order reaction (linear decay). Fick's diffusion law applies, i.e., the dispersive transport is proportional to the concentration gradient. Nitrification is the process in which nitrogen in the form of ammonia (ammoniac/ammonium) is oxidized to nitrite NO_2^- and further on to nitrate NO_3^-. Denitrification is the process in which nitrogen in oxidized form (nitrite NO_2^- or nitrate NO_3^-) is transformed into free nitrogen (N_2). This free nitrogen is released to the atmosphere.

4. Materials and methods

The 5744 ha large catchment was subdivided into 24 sub-catchments (Figure 2) based on the soil type and cover crop, as shown in Table 3. This table lists the area of each sub-catchment, the distance to the outlet, the cover crop and the main soil type. The main river, with a total

Table 3 Number, area, distance to the river outlet, main cover crop and soil type of the 24 sub-catchments in which the study basin was divided

Sub-catchment	Area (ha)	Distance to the outlet (km)	Cover crop	Soil type
1	179	22.675	Fodder beet	Loam
2	195	22.306	Maize	Loam
3	226	20.647	Maize	Loam
4	234	19.910	Maize	Loam + Silt loam
5	244	19.173	Fodder beet	Loam
6	241	17.883	Maize	Loam
7	245	17.514	Maize + Fodder beet	Loam
8	233	15.671	Maize + Fodder beet	Loam
9	247	15.302	Maize + Fodder beet + Potato	Loam
10	232	14.380	Maize + Fodder beet + Pasture	Loam
11	248	13.643	Maize + Fodder beet + Potato + Pasture	Loam
12	250	12.537	Maize + Fodder beet + Pasture	Loam
13	250	12.168	Maize + Fodder beet + Potato + Pasture	Loam
14	250	10.325	Maize + Fodder beet + Pasture	Loam
15	250	9.219	Maize + Pasture	Loam
16	250	8.482	Fodder beet + Potato	Loam
17	238	7.265	Maize + Fodder beet + Potato	Loam
18	232	5.790	Maize + Fodder beet	Loam
19	250	5.237	Maize + Fodder beet	Loam
20	250	4.776	Potato	Loam
21	250	3.670	Maize + Fodder beet	Loam
22	250	2.011	Maize + Fodder beet	Loam + Silt loam
23	250	1.289	Fodder beet + Potato	Loam + Silt loam
24	250	2.430	Maize	Loam + Silt loam

length of 23043 m, was divided into reaches with 31 nodal points, including the points of lateral inflows from each sub-catchment or block of fields and the hydraulic structures. Input data files were created for each of the sub-catchments (soil hydraulic properties, land use and other parameters). Most of the data on sub-catchment areas and river dimensions could be derived from existing databases. The drain spacing and drain depth were assumed constant at 25 m and 1.25 m below the surface, respectively for the entire region. The measured load at the outlet is equal to 107.5 kg ha^{-1} for the simulation period (four years). Daily flows and nutrient concentrations at sub-catchment level were simulated using the validated DRAINMOD and DRAINMOD-N models for the Belgian agricultural conditions (El-Sadek *et al.*, 2002c, d). The daily flows were multiplied with the nutrient concentration to obtain daily nutrient loading at the outlet of the field blocks. Nutrient load from each of the 24 field blocks was used as input to the MIKE 11 modeling code. The MIKE 11 code was run with the water quality option for a period of four years, 1990–1993. In the first approach, the exponential model was coupled with DRAINMOD, DRAINMOD-N and MIKE 11. In the second approach, MIKE 11, which includes water quality sub-model for nutrient transformation processes, was coupled with DRAINMOD field hydrology and DRAINMOD-N field water quality sub-model to develop a detailed mechanistic hydrology-water quality model.

An experimental field trial with maize, set up by the Belgian Soil Service (Coppens and Vanongeval, 1998) from 1992 to 1995, was used to calibrate and validate DRAINMOD/DRAINMOD-N model. The soil at the farm site, the Hooibeekhoeve in the community of Geel (north-eastern part of Belgium), is sandy and classified as a Haplic

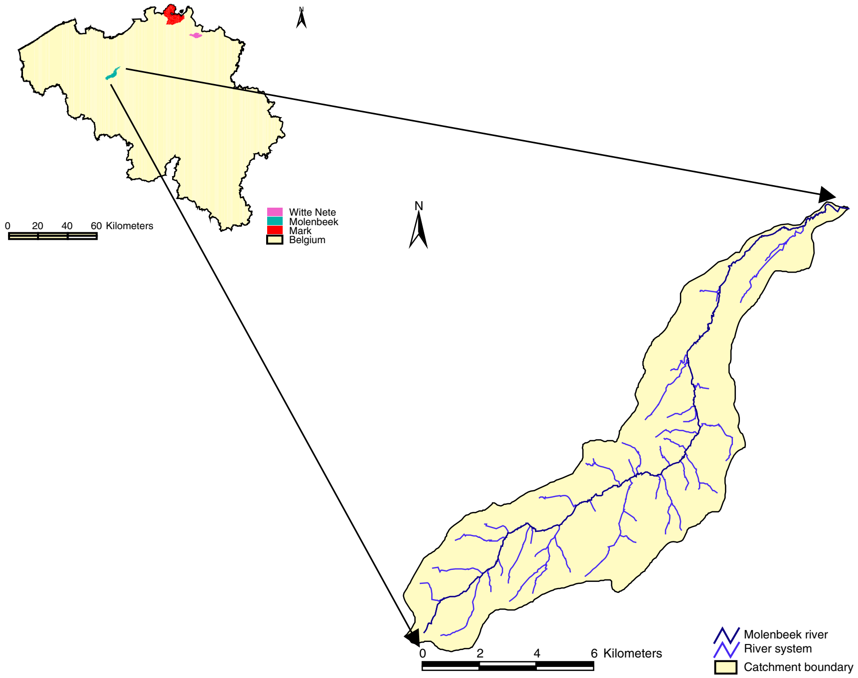

Fig. 2 The Molenbeek river basin with the delineation of the sub-catchments and the main river course

Podzol, mainly sandy soil with a distinct humus and/or iron B-horizon (a Zdg soil according to the Belgian Soil Classification System). The groundwater level fluctuates between 115 and 160 cm below surface. The first two years of the experiment, in 1993 and 1994, maize was sown, whereas in the last season, 1995, the field was fallow. Different pig slurry fertilizer application packages were applied in spring or autumn. NO_3-N in the fertilizer package is added to the soil solution by dissolution of the fertilizer. The maize production practices used in the simulations are characteristic for the sandy region of the Kempen (El-Sadek *et al.*, 2002b). Physical properties of the soil were determined in one plot of the Hooibeekhoeve for each distinguishable soil horizon, using undisturbed soil samples taken with Kopecky rings. van Genuchten-Mualem parameters for describing the hydraulic functions (van Genuchten and Nielsen, 1985) were fitted on both water retention and multi-step outflow data, using the multi-step outflow program (van Dam *et al.*, 1990). Basic water retention and hydraulic conductivity curves were established by averaging individual curves for each soil layer. The field was intensively monitored during the experimental period. Every three weeks, soil samples were taken with an interval of 30 cm to a depth of 120 cm for mineral nitrogen measurements. Mineral nitrogen was measured in groundwater at 200 cm with the same time interval. Organic manure, only as a fertilizer, was applied. Missing data, required to run the model, were either supplementary measured or reconstructed by using the transfer functions of Vereecken (1988), as indicated by Ducheyne and Feyen (1999).

4.1. Statistical analysis

The qualitative judgement of when the model performance is good is a subjective matter (Anderson and Woessner, 1992). Therefore statistical criteria are used for the quantitative judgement (Vàzquez *et al*., 2002). Statistical based criteria provide a more objective method for evaluation of the performance of the models (Ducheyne, 2000). In this study the following statistical criteria were used to evaluate the model performance:

4.1.1. Mean absolute error (MAE)

$$\mathrm{MAE} = \frac{\sum_{i=1}^{n} |(O_i - P_i)|}{n} \tag{7}$$

where O_i is the observation at time i, P_i is the prediction at time i. The MAE has a minimum value of 0.0.

4.1.2. Relative root mean square error (RRMSE)

$$\mathrm{RRMSE} = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n} (P_i - O_i)^2}}{\bar{O}\text{-}} \tag{8}$$

where $\bar{O}$ is the mean of the observed values over the time period (1 to n). The RRMSE has a minimum value of 0.0, with a better agreement close to 0.0.

4.1.3. Model efficiency (EF)

$$\mathrm{EF} = \frac{\sum_{i=1}^{n} (O_i - \bar{O}\text{-})^2 - \sum_{i=1}^{n} (P_i - O_i)^2}{\sum_{i=1}^{n} (O_i - \bar{O}\text{-})^2} \tag{9}$$

EF ranges from minus infinity to 1.0, with higher values indicating better agreement. If EF is negative, the model prediction is worse than the mean observation.

4.1.4. Coefficient of residual mass (CRM)

$$\mathrm{CRM} = \frac{\sum_{i=1}^{n} O_i - \sum_{i=1}^{n} P_i}{\sum_{i=1}^{n} O_i} \tag{10}$$

The CRM has a maximum value is 1.0. If CRM is negative the model overestimates and vice versa.

4.1.5. Coefficient of determination (CD)

$$\mathrm{CD} = \frac{\sum_{i=1}^{n} (O_i - \bar{O}\text{-})^2}{\sum_{i=1}^{n} (P_i - \bar{O}\text{-})^2} \tag{11}$$

The CD describes the ratio of the scatter of the simulated values and the observed values around the average of the observations. A CD value of one indicates to what extent the simulated and observed values match perfectly. It is positive defined without upper limit and with zero as a minimum.

4.1.6. Goodness of fit (R^2)

$$R^2 = \left[\frac{\sum_{i=1}^{n} (O_i - \bar{O}^-)(P_i - \bar{P}^-)}{\sqrt{\sum_{i=1}^{n} (O_i - \bar{O}^-)^2} \sqrt{\sum_{i=1}^{n} (P_i - \bar{P}^-)^2}} \right]^2 \tag{12}$$

where $\bar{P}$ is the mean of the predicted values over the time period (1 to n). R^2 is ranging from 0.0 to 1.0 indicating a better agreement for values close to 1.0 and it is known as the goodness of fit (Shahin *et al.*, 1993; Legates and McCabe, 1999; Vàzquez *et al.*, 2002).

5. Results

5.1. DRAINMOD/DRAINMOD-N calibration and validation

A 3-year time series of data (1992–1995) of the Hooibeekhoeve in the community of Geel was used to calibrate and validate the DRAINMOD/DRAINMOD-N models. The soil, crop and nitrogen parameters were calibrated resulting in a set of representative parameters for the given soil-crop condition. The calibration of the model parameters was carried out by trial and error (Loague and Green, 1991). The calibration of DRAINMOD-N model is based on field data of the fertilizer scenario of 30 ton ha^{-1} pig slurry applied in spring (Figure 3). The calibrated model (DRAINMOD-N) was validated versus data collected on the field fertilizer scenario of 60 ton ha^{-1} pig slurry applied in autumn + 60 ton ha^{-1} pig slurry applied in spring (El-Sadek, 2002a). Finally, the calibrated and validated model was applied to simulate the nitrate transport in the soil profile for the other scenarios (30 ton ha^{-1} pig slurry applied in autumn, 120 ton ha^{-1} pig slurry applied in autumn and 120 ton ha^{-1} pig slurry applied in spring). Summary of inputs and calibrated parameters of the DRAINMOD/DRAINMOD-N model in the Hooibeekhoeve field is shown in Table 4. Validation results are shown in Figure 4. The calibrated and validated DRAINMOD/DRAINMOD-N models were used to assess the nitrate-nitrogen leaching from the 24 sub-catchments in which the river Molenbeek basin was subdivided. In the scenario-analysis, it was assumed that the field blocks were equipped with a subsurface drainage system consisting of parallel, 10 cm diameter, corrugated plastic drains, situated at a depth of 1.25 m below surface and 25 m spaced.

5.2. MIKE 11 calibration

The hydrologic module in MIKE 11 (NAM) was calibrated for two different parameter groups: first the parameter of the transport models (the recession constants or time constants for baseflow, for interflow and for overland flow). Secondly the water balance parameters (maximum water content in the lower zone storage $L_{\max}$, maximum water content in the surface storage $U_{\max}$, and overland flow runoff coefficient). To enable testing if the NAM module is properly simulating baseflow, interflow and runoff, a recursive digital filter was applied (Willems, 2000; Nathan and McMahon, 1990; Chapman, 1991) to separate total flow in three subflows. The working-principle of the filter can be explained physically as the routing of a high frequency signal through a linear reservoir, with the reservoir constant

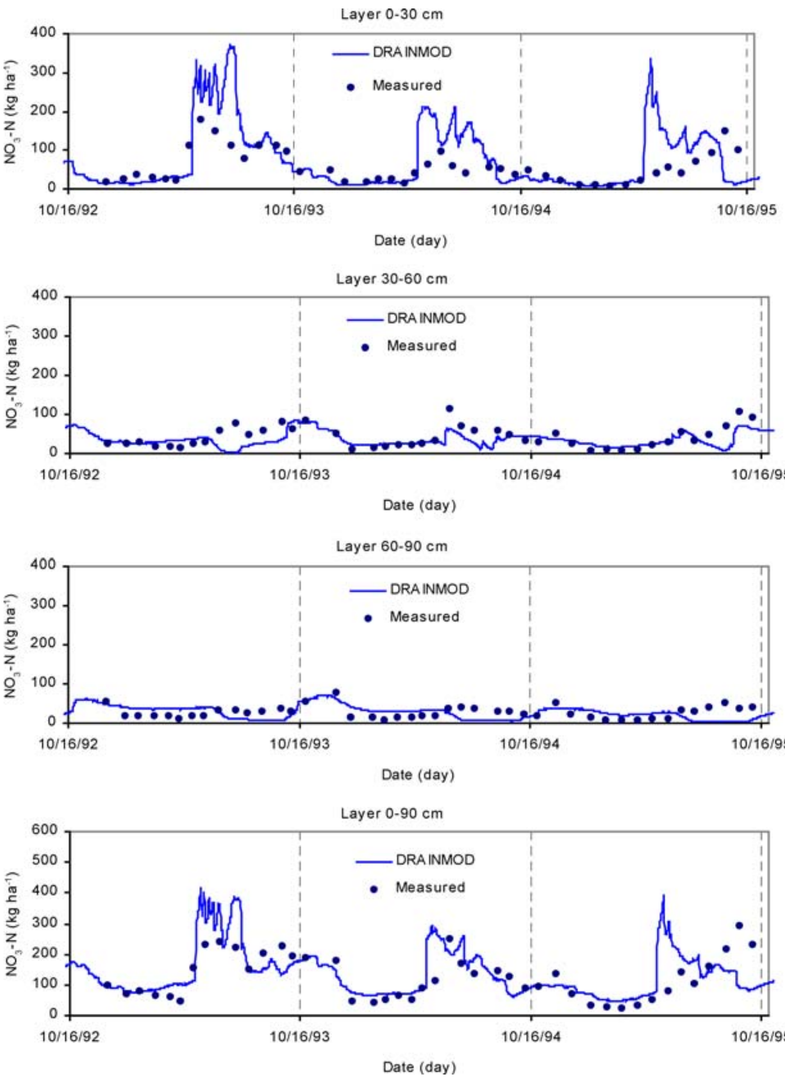

Fig. 3 NO_3-N content in the soil profile at different depths in maize field and sand soil in Geel using fertilizer application of 30 ton ha^{-1} (pig slurry)

equal to the recession constant of the signal that is filtered. In this reservoir routing, the routed signal is considered equal to the filtered signal as it has the same qualitative behavior in recession periods. The subflows with the largest recession constants are separated first. In that way, baseflow is first separated from total rainfall-runoff discharges, secondly interflow is separated from total discharges of surface runoff and interflow. Finally, total flow filtered series is the sum of the three filtered subflows. As time series are often disturbed by random fluctuations that are introduced by the river system (e.g. by regulating structures), the filter is used to get rid of these random fluctuation (Figure 5). The recession constants (time constants) of the subflows are calibrated as the average value of the inverse of the slope of the linear path in the recession periods of a Log (Q) – time graph for the three subflows.

Table 4 Summary of inputs and calibrated parameters in the Hooibeekhoeve

Soil properties	
θ_{wp} (cm^3 cm^{-3})	0.17
Bulk density (g cm^{-3})	1.6
Organic nitrogen in top soil (μg g^{-1})	3200
K_{mnl} (d^{-1})	3.5×10^{-5}
K_{den} (d^{-1})	0.01
Drainage system parameters	
Drain depth (m)	1.25
Drain spacing (m)	25
Surface storage (cm)	2.5
Effective drain radius (cm)	2.5
Maize production parameters	
Desired planting date	May 4
Length of growing season (d)	120
N-fertilizer input (kg N ha^{-1})	160
Date fertilizer application	May 6, May 14
Depth fertilizer incorporated (cm)	10
Total dry matter production (kg ha^{-1})	14500
Other nitrogen model parameters	
Dispersivity (cm)	10
NO_3-N content of plant (per cent)	1.55
NO_3-N concentration of rain (mg l^{-1})	0.8

Calibration of the water balance parameters (maximum water content in surface storage U_{max}, maximum water content in root zone storage L_{max}, and overland flow runoff coefficient) are done by trial and error. The procedure is repeated till the maximization of the agreement between the measured and modeled peak discharges and total volumes is achieved. During the calibration procedure of the water balance parameters, the models are evaluated in three steps:

1. *Evaluation of water balance* (*comparison of simulated and observed runoff volumes*) by plotting cumulative simulated and measured runoff for the full time series (Figure 6).
2. *Evaluation of peak flows and low flows* (*comparison of hydrograph maxima and minima for the different individual rain storms*).
   For such evaluation, the time series is divided into two types of storm periods: first for individual storm events (containing individual hydrograph peaks), and secondly for longer events of shortly successive rain storms (containing a baseflow recession periods of minimum length). The comparison is done by plotting the maximum of each peak and the minimum of each event for both measured and simulated time series as shown in Figure 7 for peak flows, and Figure 8 for low flows. As the plotted points are close to the bisector, the comparison between measured and simulated values is good.
3. *Evaluation of long-term statistics.*
   The observed and simulated discharge values in the full time series are plotted after ranking them in an ascending order (Figure 9). The flattening of the measurement curve is explained by river flooding (which starts at 6 m^3 s^{-1} at station 20). As flooding is described by the hydrodynamic model and not by the hydrological model, these discharges should not be taken into account during the NAM calibration.

The total length of the Molenbeek brook is approximately 23 km. For the first 6 km no detailed data about cross-sections and hydraulic structures are available, but for the next

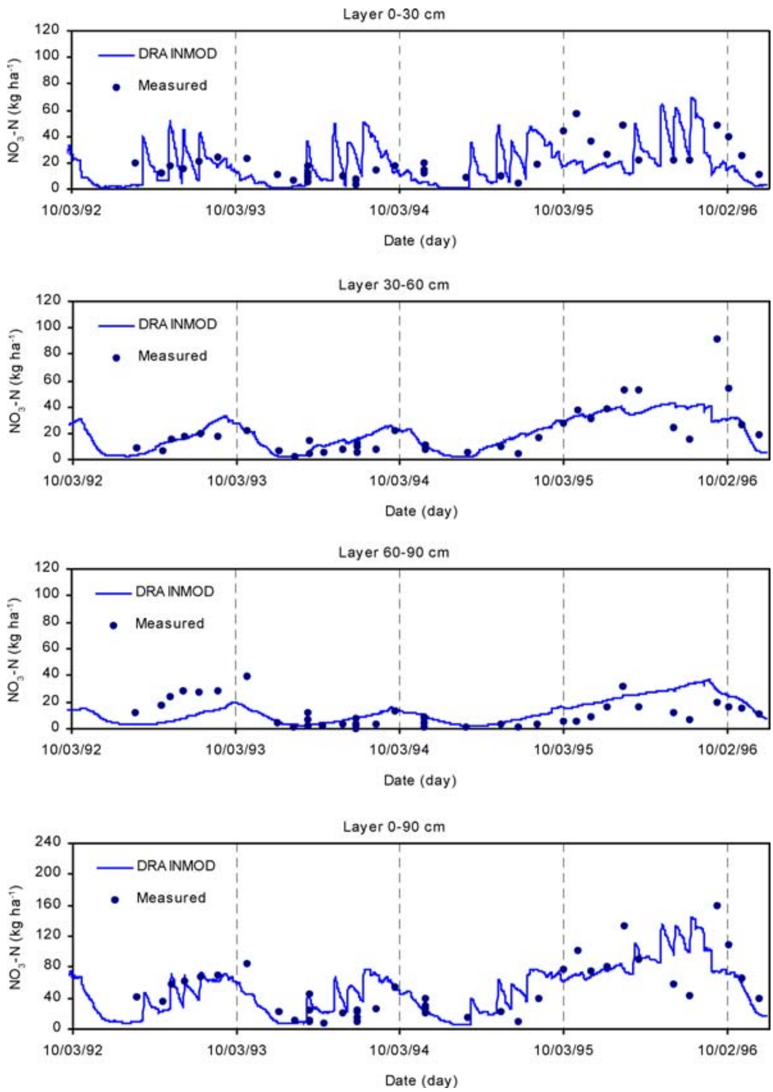

Fig. 4 NO_3-N content in the soil profile at different depths in pasture field and sand soil in Geel using fertilizer application of 20 ton ha^{-1} (cow slurry)

17 km, detailed data about cross-sections and all-important hydraulic structures exist. The latter cross-sections are 440 in total. In this way, the variation in channel geometry along the model branches can be described adequately. For the structures, all 16 bridges, 16 weirs, 6 culverts and 6 control structures over the distance of 17 km are considered. The 6 control structures regulate the water levels at different locations along the brook to prevent areas from flooding, and to limit the flow velocities to avoid erosion of the riverbed. After implementation of the HD model, the simulation result is compared with the measurements at Mere station. More specifically, the simulated Q-H is compared with the measured. The results shown in Figure 10 indicate that the dynamics of the system are presented well.

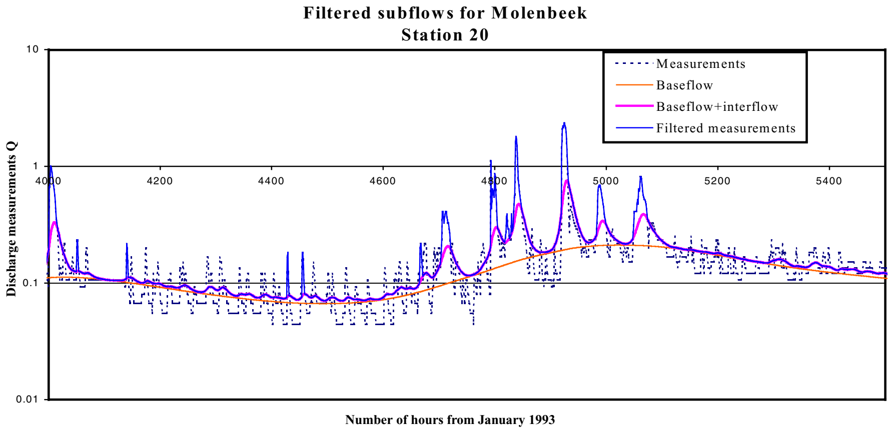

Fig. 5 Splitting of the total discharge of the river Molenbeek in base flow, interflow and runoff

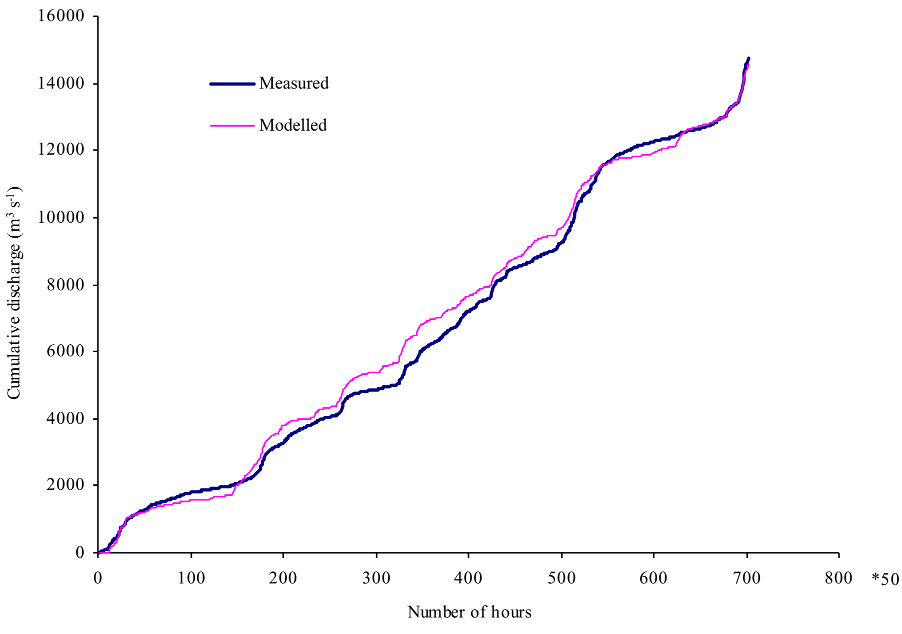

Fig. 6 Comparison between cumulative measured and simulated discharges

The water quality model was calibrated by trial and error to obtain a reasonable fit between the measured and the modeled results. Initial values for the parameters of the process equations are based on standard values found in literature (Brown and Barnwell, 1987; DHI, 1998). Certain parameters are strongly dependent on the location. The calibration was difficult because of the long interval between each of the measurements of the Flemish Environmental Agency (minimum one month). The only parameter calibrated is the nitrification decay coefficient.

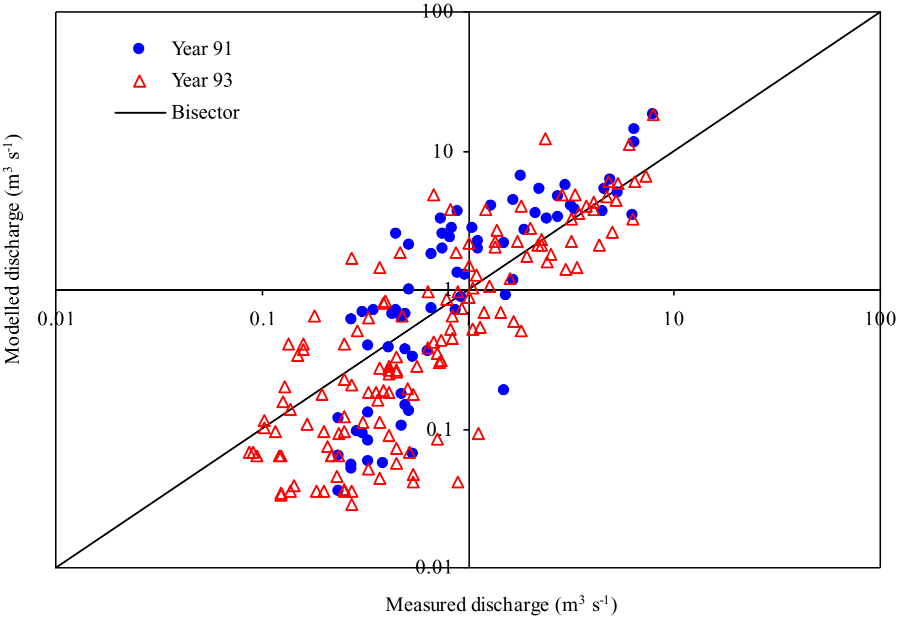

Fig. 7 Comparison between measured and simulated values for maximum of each peak

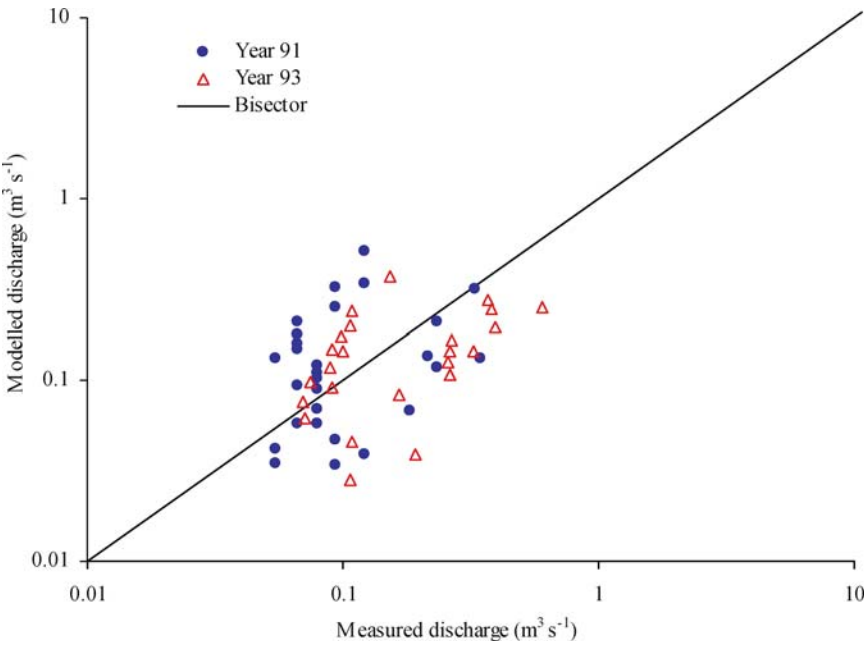

Fig. 8 Comparison between simulated and measured values for minimum of each event

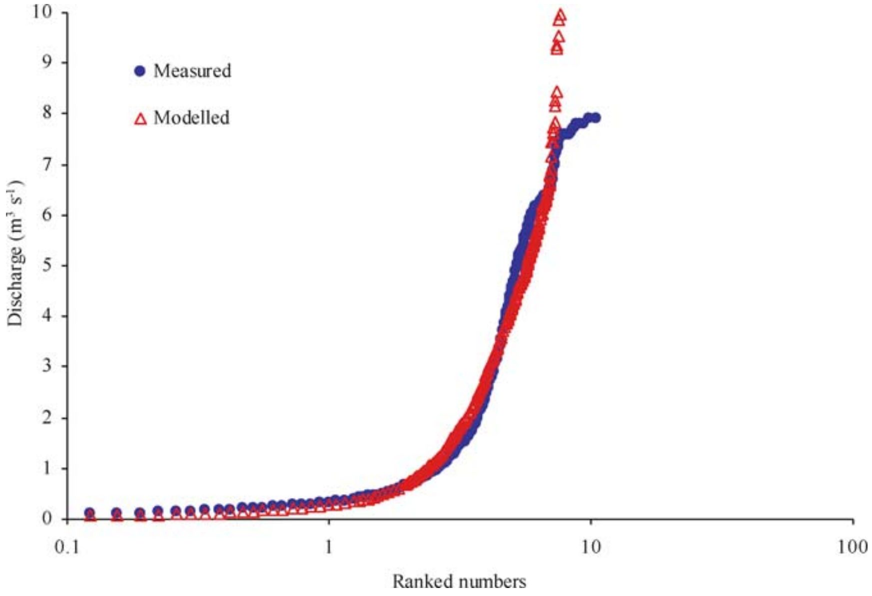

Fig. 9 Comparison between measured and simulated values

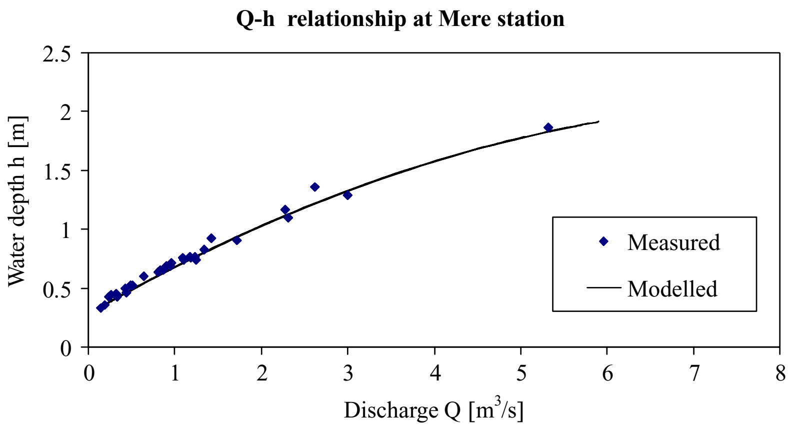

Fig. 10 Simulated and measured Q-H relationship at mere station

6. Discussion

The validated MIKE 11 (Radwan *et al.*, 2000) was run with a 4-year data set to simulate daily flow velocities at all nodes in the river. It was found that average velocity is a function of the season. In general, the wet season had higher velocities. The large velocities occurred infrequently due to larger summer storms. The travel time was estimated as a function of distance from the field edge to the catchment outlet assuming average velocity throughout the catchment. The validated MIKE 11 (using DRAINMOD flow as input) was used to calculate the velocity-input file to the lumped exponential model. MIKE 11 and DRAINMOD outputs of daily discharge rates at Mere station in the Molenbeek catchment were verified using

Table 5 Annual measured and simulated NO_3-N load, in kg ha^{-1}, at the river outlet, for the period 1990–1993

Year	Measured	Simulated with exponential model	Simulated with MIKE 11
1990	2.6	4.0	8.8
1991	40.1	29.8	31.7
1992	17.8	22.4	17.1
1993	47.0	65.6	36.8

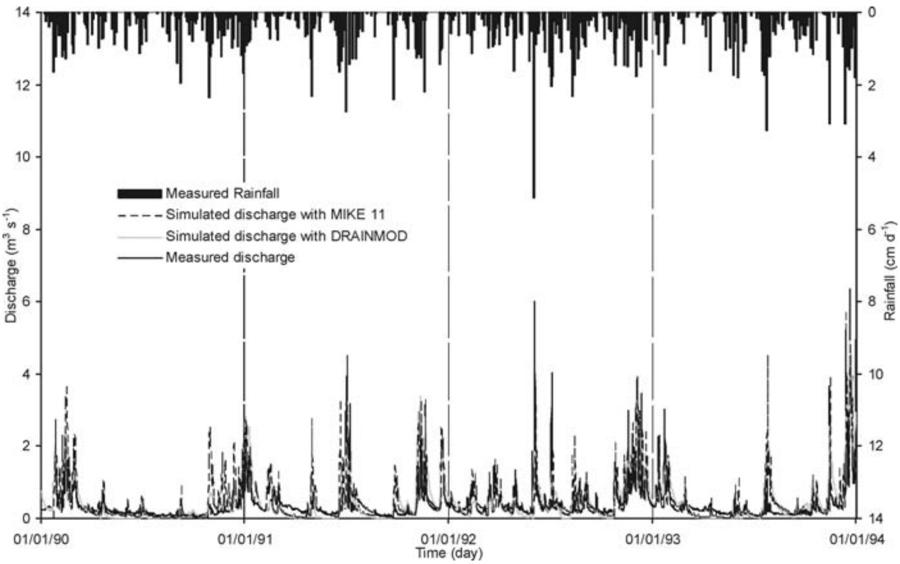

Fig. 11 Daily precipitation, observed and simulated daily discharge at the outlet station for the period 1990–1993

measured data as shown in Figure 11. The nutrient loading or concentration at the edge of a field is simulated using DRAINMOD-N. The predicted discharge outflows are used with a flow-weighted concentration to obtain N loadings at the individual outlets of the fields with different management scenarios. The annual measured and simulated NO_3-N load, in kg ha^{-1}, at the river outlet is given in Table 5 and a comparison of total simulated nitrate load from all fields versus measured data is shown in Figure 12.

Concentration peaks within the period of fertilizer application between March and May can be clearly seen in years 1991, 1992 and 1993. The nitrate load peaks correspond to the rainfall events in these years. This occurs as the upper layers of the soil become saturated allowing the fertilizer to dissolve in the available moisture and to be transported to the river. The low load in 1990 is the result of a dry year. The agreement between the measured and predicted nitrate load in Table 5 and Figure 12 is good. However, it is recognized that daily time series output cannot be compared in detail against monthly point measurements. Plants take approximately 60% of the applied nitrogen with 30% transported via groundwater and surface waters to the river. The time series with predominantly agricultural influences showed the expected winter maximum and summer minimum. The effect of the strong influence of previous year values on the present year can be seen in Table 5 and the time series of the cumulative nitrate load given in Figure 12. The effect of season on the nitrate

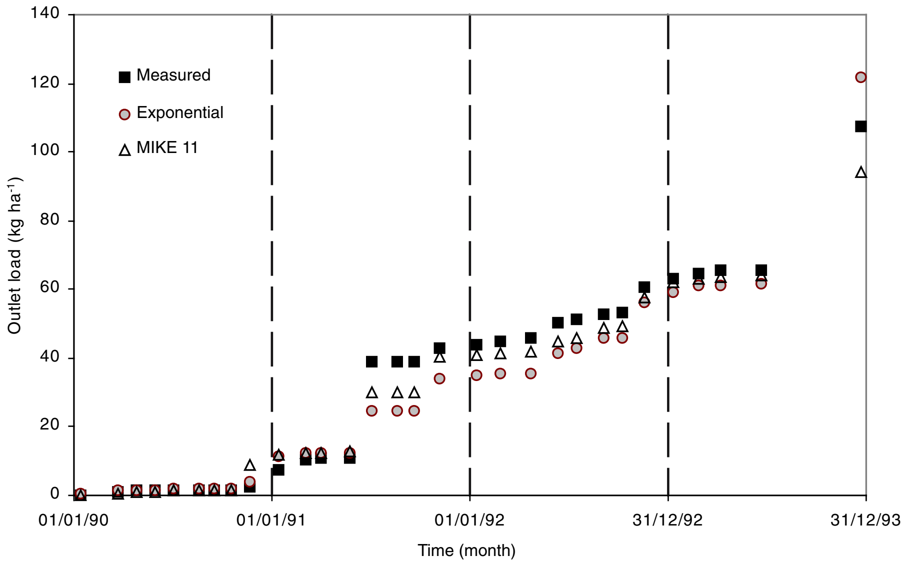

Fig. 12 Predicted and measured cumulative nitrate load at the outlet station for the period 1990–1993

load can be seen in this figure. The residual concentrations in summer tend to have negative effects whereas corresponding concentrations in the winter still have positive effects. This means that the effect of the previous year differs depending upon the rainfall time series. High levels of nitrate in a preceding winter have the effect of lowering concentrations in the following summer. Equally the effects of low values in a preceding summer increase the nitrate concentrations in the following winter. The winter-summer difference in annual nitrogen cycle at the catchment outlet compensates the difference in the following season. For example, in 1992, the difference in nitrate load of the winter season is compensated by the winter-summer difference in annual nitrogen cycle. A wet winter could act to flush out reserves of nitrate leaving little that could be readily removed in the subsequent summer. For example, a dry summer leads to storage of readily mineralizable nitrogen, once the soils wet up again this large reserve of nitrogen stimulates the microbial population to increased activity that enhances nitrate leaching the following winter. The increased microbial activity tends to remove more of the available nitrogen than was preserved from previous summer.

In general, modeling nitrate export purely in terms of the export from present land use tends to overestimate nitrate loads. It is uncertain how much of the nitrate moves directly to the streams in the catchment without going via groundwater. It certainly occurs in the study area, although it seems that the link between soil nitrogen reserves and both river and groundwater is a straightforward. The comparative analysis reveals that both the lumped (exponential model) and the MIKE 11 model are able to simulate with acceptable accuracy the monthly NO_3-N load at the catchment outlet for the 1990–1993 period. The statistical analysis results presented in the Table 6 clearly illustrate that on average DRAINMOD-MIKE 11 model performs better in the prediction of the NO_3-N load at the catchment outlet. The study revealed that for the lumped exponential model the initial field load is the most significant input. Based on published values, a value of (K) (0.10) for nitrate-nitrogen gave reasonable results. A smaller value of (K) may be used for very wet seasons compared to dry seasons. MIKE 11 can estimate travel time using simulated velocity data. The lumped parameter water

Table 6 Statistical performance analysis calculated for the simulation period 1990–1993 for monthly NO_3-N loads

	MAE	RRMSE	CD	EF	CRM	R^2
Measured & Exponential (lumped)	1.941	1.309	0.640	0.713	−0.133	0.831
Measured & DRAINMOD-MIKE 11	1.668	0.963	1.930	0.845	0.123	0.900

MAE: mean absolute error; RRMSE: relative root mean square error; CD: coefficient of determination; EF: model efficiency; CRM: coefficient of residual mass; R^2: goodness of fit

quality model as discussed in this study has to be tested and validated in different locations. Testing of this parameter model is challenging but necessary for agricultural lands with complex land management practices. More field experiments and studies may be required to determine the decay parameter (K) for other nutrients. A large effort should be placed on obtaining its accurate determination and statistical distribution. The lumped (exponential) approach relies on data from readily available databases. The model has relatively few data requirements, and can be easily calibrated, providing a relatively inexpensive, robust means of evaluating the impact of land use and land management on water quality for modeling on an annual basis. The approach reduces the problems inherent in predicting the nitrate load on a daily basis. Another limitation on the use of these models is that the importance of hydrological pathways in determining nutrient delivery to surface waters, and the variations in available transport mechanisms over annual water cycle mean that the models can not predict in real time. Therefore, the approach can be used to predict on a year-by-year basis, the changes in water quality within the catchment.

7. Conclusions

Two approaches, the MIKE 11-DRAINMOD and the lumped, exponential based distributed catchment scale hydrologic and water quality model were tested using four years of measured data of the Molenbeek catchment, Belgium. The modeling approaches were applied in a distributed way and used to model the nutrient load in the river Molenbeek. The statistical analysis indicated that the two approaches are able to reconstruct quite accurately the nitrate load of a primarily agricultural catchment with heterogeneous land management practice. For the analysis the catchment was subdivided in 24, more or less homogeneous, sub-basins with a particular soil-land use management practice. The MIKE 11 prediction of in-stream flow rates (velocities and depths) indicated the potential of the model for being coupled with the DRAINMOD-N model and the Exponential model for predicting cumulative water quality impacts on the Molenbeek catchment. The comparative analysis between both model approaches (lumped and DRAINMOD-MIKE 11) reveals that the lumped model is able to predict sufficiently accurate nutrient load at the catchment outlet. The complex approach (DRAINMOD-MIKE 11) however has the advantage of giving a more accurate estimate of the nutrient load at the catchment outlet, resulting in a more precise modeling of the nutrient load transport and transformation in the land phase and the river of catchments. As such the approach can be used to derive for the study area the fertilizer practice that will result in a NO_3-N load at the river outlet that does not exceed the limits, as specified by environmental considerations. When measured data are not available, calibrated and validated DRAINMOD in Flanders, Belgium could be used to predict water discharges. Efforts should be made to validate DRAINMOD-N for agriculture fields on the poorly drained soils in Belgium. More field studies and experiments are needed in determination nutrient decay parameter for the

Exponential models. Since such models have relatively few data requirements, and can be easily calibrated, they will be the suitable tools to model the total nutrient load at the catchment outlet when Geographic information system (GIS) facilities are not available.

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