*Intl. J. River Basin Management* Vol. 1, No. 2 (2003), pp. 97–103


# Modelling of dissolved oxygen and biochemical oxygen demand in river water using a detailed and a simplified model

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**ABSTRACT**

Different model types are available to model catchment surface water quantity and quality. They vary from detailed physically-based models to simplified conceptual and empirical models. The most appropriate model type for a certain application depends on the project objectives and the data availability. The detailed models are very useful for short-term simulations of representative events. For long-term statistical information and as a management tool they cannot be used. For that purpose more simplified (conceptual or meta) models have to be used. In this study, dissolved oxygen (DO) and biochemical oxygen demand (BOD) dynamics are modelled in a river in Flanders. BOD sources from agricultural leaching and domestic point sources are considered. Based on this input, concentrations of DO and BOD in the river water are modelled in Mike11 (river modelling software from DHI Water & Environment). Advection and dispersion were taken into consideration, together with the most important biological and chemical processes. Model calibration was done on the basis of available measured water quality data. A more simplified model was calibrated to this detailed model, with the objective to yield more easily long-term simulation results which can be used in a statistical analysis. Two aspects of adequacy of model results are highlighted, namely accuracy and model speed. The conceptual simplified model is 1800 times faster than the Mike11 model. Moreover, the two models have almost the same accuracy. The construction of the simplified model is, however, only possible using simulations with the detailed model. The detailed and the simplified model have to be used in a complementary way.

*Keywords*: Water quality modelling; simplified model; sensitivity analysis.

## Introduction

Planning and management activities require the assessment of hydraulic and water quality conditions often beyond the range of observed field data. In this context both hydraulic and water quality models must be formulated that are general enough to (1) describe observed conditions; and (2) predict planning scenarios that may be substantially different from observed conditions. In stream water pollution control, the main objective is to assess if the system complies with the maximum pollutant releases, allowed from point and nonpoint source pollution, so that pollutant levels in the receiving streams meet the water quality standards. Water quality models for in stream water pollution control have been calibrated and verified with data collected prior to model development during surveys designed to check basinwide water quality for regulatory compliance (Melching and Yoon, 1996). These data are typically inadequate for the following reasons:

- Many key water quality constituents or inputs are not measured because the purpose of the data collection is a general survey of water quality conditions in the stream system and not the development of a water quality model;
- There is tendency to sample certain water quality constituents because they are easy to sample, not because they increase knowledge of key water quality processes (Reckhow, 1979); and
- The frequency of data collection is usually insufficient.

These inadequacies force water quality modellers to make weakly supported assumptions regarding model parameters or inputs, and to use simplified model descriptions that require less input and parameters. Thus model prediction uncertainty increases and decision making for water pollution control is adversely affected.

In this study the sensitivity is analysed for two water quality models which are different in the level of complexity of the modelled processes. The evaluation is based on the following two aspects: the accuracy of the model results and the model speed.

## Dissolved oxygen and biochemical oxygen demand

### *General information*

Dissolved oxygen (DO) refers to the volume of oxygen that is contained in water. Oxygen enters the water by photosynthesis

Received and accepted on May 19, 2003. Open for discussion until September 30, 2003.

of aquatic biota and by the transfer of oxygen across the air–water interface. The amount of oxygen that can be held by the water depends on the water temperature, among other variables as described in Smith (1990).

Once absorbed, oxygen is either incorporated throughout the water body via internal currents or is lost from the system. Flowing water is more likely to have high dissolved oxygen levels than is stagnant water because of the water movement at the air–water interface. In flowing water, oxygen–rich water at the surface is constantly being replaced by water containing less oxygen as a result of turbulence, creating a greater potential for exchange of oxygen across the air–water interface.

*Environmental effects*

The introduction of excess organic matter may result in a depletion of oxygen from an aquatic system, mainly during warm, stagnant conditions that prevent river water mixing. Prolonged exposure to low dissolved oxygen levels ($<$5–6 mg/l) may not directly kill an organism, but will increase its susceptibility to other environmental stresses. Exposure to $<$30% saturation ($<$2 mg/l oxygen) for one to four days may kill most of the biota in a system (Gower, 1980).

*DO–BOD cycle in river water*

In Figure 1 the most important processes involved in modelling DO are shown in a schematic way. Oxygen in the aquatic environment is produced by photosynthesis of algae and plants and consumed by respiration of plants, animals and bacteria, BOD degradation process, sediment oxygen demand and oxidation. It is re-aerated through interchange with the atmosphere. These processes are considered for the modelling in this study.

In Figure 2, a schematic overview is given of the most dominant processes related to the modelling of BOD. Degradation of the organic matter expressed as BOD gives rise to an equivalent consumption of oxygen. Degradation of BOD is also a source of nutrients ($NH_4$-N) that can be oxidized and that gives rise to an additional oxygen consumption.

*Modelling system Mike11*

The water quality (WQ) module of Mike11 has been developed by DHI Water & Environment. This module deals with the basic

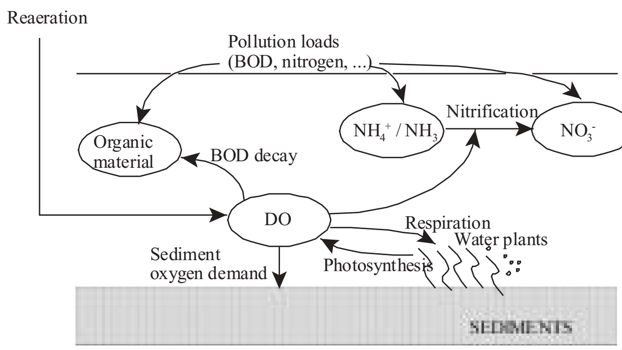


Figure 1 Processes related to the modelling of DO.

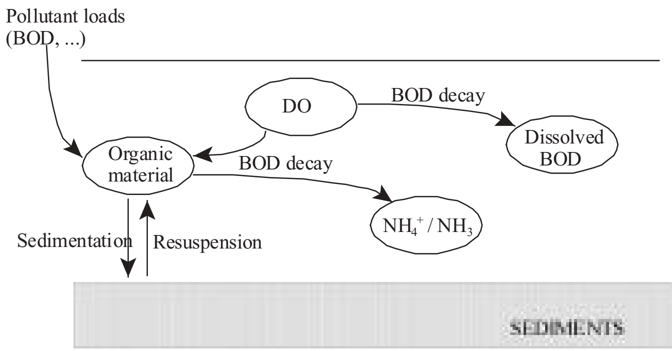


Figure 2 Processes related to the modelling of BOD.

aspects of river water quality in areas influenced by human activities such as oxygen depletion and ammonia levels as a result of organic matter loading. The WQ module is coupled to the advection–dispersion (AD) module, which means that the WQ module deals with transforming processes of compounds in the river and the AD module is used to simulate the simultaneous transport process. The WQ module solves the system-coupled differential equations describing the physical, chemical and biological interactions in the river. The river water quality can be dealt with at different levels of detail (model levels from 1 to 6). In this study, model level 4 has been chosen. This means that BOD–DO relationships include exchange with the river bed and nitrification and denitrification. At this level, concentrations of dissolved oxygen (DO), biological oxygen demand (BOD), ammonium ($NH_4$-N) and nitrate ($NO_3$-N) are computed in Mike11 by taking into consideration advection–dispersion and the most important physical, chemical and biological processes. The description of these processes can be found in the Mike11 reference manual (DHI, 2002).

The processes are described with process velocities of 1st order ($dC/dt \sim C$), the dependence on temperature with Arrhenius terms ($\ln(dC/dt) \sim T$, with T the temperature of the river water, and C the modelled concentration). The process deceleration at low concentrations is modelled with Monod terms ($dC/dt \sim K/(K + C)$). This way of presenting the processes is called macroscopic, because it tries to represent the way they are observed macroscopically with equations. The different processes on the microscopic scale that form the basis of the macroscopic observation are thus not considered.

## Case-study

*Study area*

The study was carried out for the Molenbeek brook, which is one of the main tributaries of the river Dender in Belgium. The hydrographic catchment of the Molenbeek has an area of 57.44 km$^2$. It has one limnigraphic station at the village of Mere at which the total upstream area equals 40.5 km$^2$ (Figure 3).

*Input data and models*

Along the Molenbeek brook, the major sources of pollution are agricultural drainage, industrial and domestic waste water.

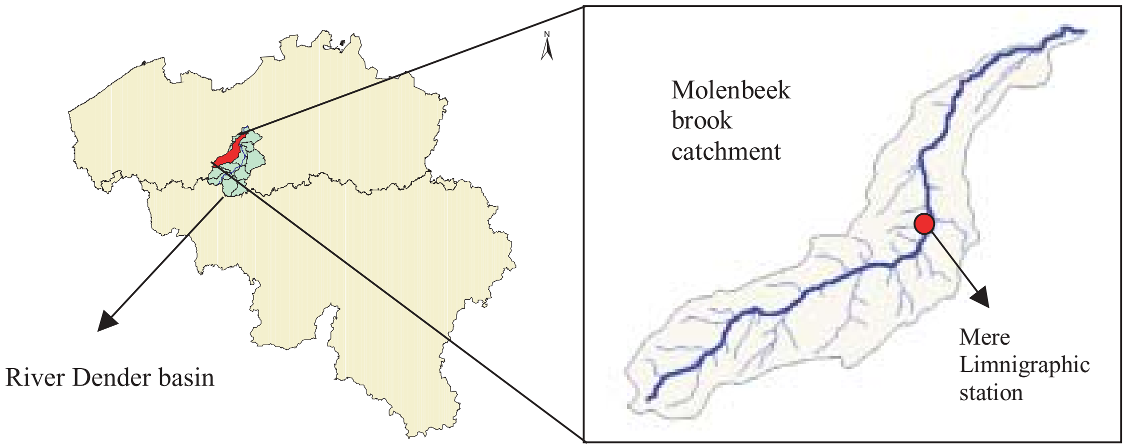


Figure 3 Plan view of the Molenbeek brook catchment, together with the localization within the larger river Dender basin and Belgium.

Agricultural activities in the catchment are about 76% of the total area. To estimate nitrate leaching, a DRAINMOD-N model (Brevé *et al.*, 1997) is used. A detailed description of each functional relationship and a model application in the Netherlands and Flanders is given by El-Sadek *et al.* (2000). Its application for the Molenbeek brook is given by Radwan *et al.* (2000). The climates, soil, crop and crop management data, required as input for the water and nitrate transport modelling, were collected. The distributions over the catchment of the model input and simulation results were presented graphically using GIS. Combination of soil type and the main agricultural land units resulted in 32 scenarios, being the result of eight soil types and four main field crops. The soil–land use map was overlaid by the parcel map and for each parcel the climate, soil, crop conditions and nitrogen application depth were determined and used as input for the DRAINMOD model. The leaching period from 1 January 1990 to 31 December 1997 was simulated using the measured $NO_3$-N concentrations on 16 December 1989 as the initial condition. The simulation results are used as input for Mike11.

There are 21 sewerage outlet pipes along the Molenbeek brook which receive untreated domestic wastes. For each point, the total population discharging to it is calculated (VMM, 1995) and then the concentration of untreated effluent was evaluated by assuming concentrations of BOD and ammonia equal to 54 and 10 g/capita day (VMM, 1992).

The industrial wastes are considered to be one of the main sources of water pollution because of their toxic chemicals and organic loading. There is one factory in the studied catchment. The pollution load from this factory is estimated for the different water quality variables on the basis of measurements of the Flemish Environmental Agency (VMM) and assumed constant in time.

### *Model calibration*

Calibration of the water quality model parameters (process rates and Arrhenius terms) could not be done because of the limited time resolution of the available immission measurements. Only for the nitrification decay coefficient, rough calibration could be performed. When the leached $NO_3$-N concentrations (as input for Mike11, see previous section) were simulated in the Mike11 model using the default values for the nitrification decay coefficient, bad qualitative agreement (in terms of the time evolution of the concentrations) was observed with the $NO_3$-N measurements in the river. This could not be fully explained by the possibility of quantitative overestimations in the $NO_3$-N input. Therefore, it was concluded that the default value for the coefficient is quite high and that the $NO_3$-N concentrations are increased too much due to the high nitrification process velocity. The value was reduced from 1.54/day to 0.54/day which gives also the best fit with the $NO_3$-N measurements in the river water. The default parameter values in DHI (2002) were used for all other parameters.

## Conceptual simplified model

### *Concept*

The significance of different water quality processes varies depending on the case study considered. Only the most important processes were considered because of the large limitations in the available data. A sensitivity analysis was carried out to evaluate the different water quality processes. Based on the results, a simplified river water quality model was set up. In this simplified model, advection and dispersion are modelled using a linear reservoir model (recession constant for the dispersion and time lag for the input to the reservoir for the advection). Both parameters are calibrated based on simulations with the Mike11 model by only considering advection–dispersion. During the residence time of the water in the reservoir, only the most dominant water quality processes are modelled. This is done in a simplified way using "concentration reduction factors". For calibration of these factors, two simulations are carried out with the Mike11 model. In the first simulation, only the advection–dispersion processes are considered, while in the second simulation the water quality processes are also included. By comparing the results of the first and the second simulation, the concentration reduction factors $f_{DO}$ and $f_{BOD}$ are derived. More details on the calibration of the simplified conceptual model can be found in Willems (2000).

*Sensitivity analysis of water quality processes*

The aim of the sensitivity analysis is to estimate the rate of change in the output of the model with respect to changes in the model inputs and/or model parameters. Such knowledge is important for (a) evaluating the applicability of the model, (b) determining parameters for which it is important to have more accurate values, and (c) understanding the behaviour of the system being modelled. A sensitivity analysis is carried out for the different water quality processes and parameters to assess the most sensitive parameters/processes for the purpose of river quality management and monitoring plans.

A comparison is made between the simulation results by using default parameter values and a simulation in which the parameter values are drastically changed. The change in the simulation results is presented by the concentration reduction factor $f$ which is plotted for all modelled pollutants. Based on the results, the processes which affect the results in a significant way are considered in the conceptual simplified model. For the implementation of these processes, the same process equations are considered in both models. The processes examined by the sensitivity analysis are: nitrification, BOD decay, photosynthesis, respiration and reaeration. Two examples of studied sensitivities for the case-study of the Molenbeek river in Belgium are presented in Figures 4 and 5. Hydrological and hydrodynamic results are described elsewhere in Radwan *et al.* (1999, 2000).

In Figures 4 and 5, no unique relationship is found between the concentration reduction factor and the temperature because different processes considered in the Mike11 model have an influence on the reduction factor. This means that the reduction factor is not only depending on the temperature, but also on the pollutant concentrations modelled. Therefore, Figure 4 cannot be used to calibrate the concentration reduction factors. It is only used to check the sensitivities of the different processes and to check the importance of having processes included in the simplified model. It is clear that the conclusions derived from this analysis are strongly depending on the specific case considered (the local conditions). When the model is used for another river, a different detailed model will be implemented, and also the conceptual model has to be identified and calibrated again. Such recalibration might even be needed when other management scenario's are considered for the same river.

*Simplified model structure*

For the Molenbeek case-study, the following simplified river model is derived (using the concentration reduction factors $f_{DO}$ and $f_{BOD}$ as defined before):

$$f_{DO} = 1 + \left(\frac{dDO}{dt}\right) T_r$$

$$f_{BOD} = 1 + \left(\frac{dBOD}{dt}\right) T_r$$

where $T_r$ is the residence time.

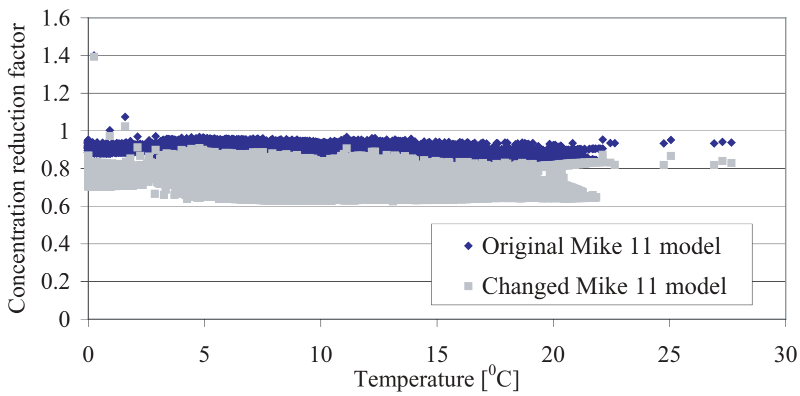


Figure 4 Influence of an increase in BOD degradation rate (from 0.5 to 1.5/day) on the concentration reduction factor for BOD.

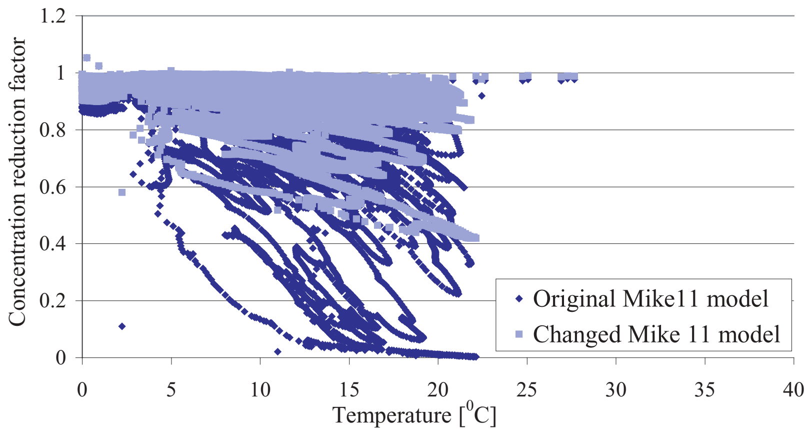


Figure 5 Influence of a decrease in the nitrification rate (from 0.54 to 0.3/day) on the concentration reduction factor for DO.

The sensitivity analysis shows that, the main processes affecting the DO concentration are the nitrification and the BOD degradation processes. For BOD, the main process is the BOD degradation process. By considering only these processes, the previous equations are written as follows:

$$f_{DO} = 1 - \left( k_{\deg rad} \frac{BOD}{DO} \theta_{\deg rad}^{T-20} + y_{nitr} k_{nitr} \frac{NH_4\text{-}N}{DO} \theta_{nitr}^{T-20} \right) T_r$$

$$f_{BOD} = 1 - k_{\deg rad}\, \theta_{\deg rad}^{T-20} T_r$$

*Results and discussion*

The Mike11 model and the conceptual simplified model were simulated for a period of 8 years. Observed flows, rain and temperature data for the period 1990 to 1997 were hereby used. The calculations were performed on an hourly basis. In Figures 6 and 7, the simulation results are compared with the observations for a complete simulation period of 7 years. The first year of the total simulation period of 8 years was excluded from the simplified model results because of the inaccurate influence of the initial conditions. The figures indicate that the general performance of the two models is satisfactory in terms of the magnitude of the concentrations and its variability in time. This means that the long-term statistics of the modelled concentrations seem to be realistic. For specific time moments, however, the model shows important over- and underestimations of the concentrations. This is due to many uncertainty sources involved in the modelling process. Apart from the parameter calibration, uncertainties also arise from the rainfall input estimation, the hydrological model of the river catchment, the hydrodynamic river model, the input of the different pollution sources, and the structure (process schematisation) of the two types of water quality models considered.

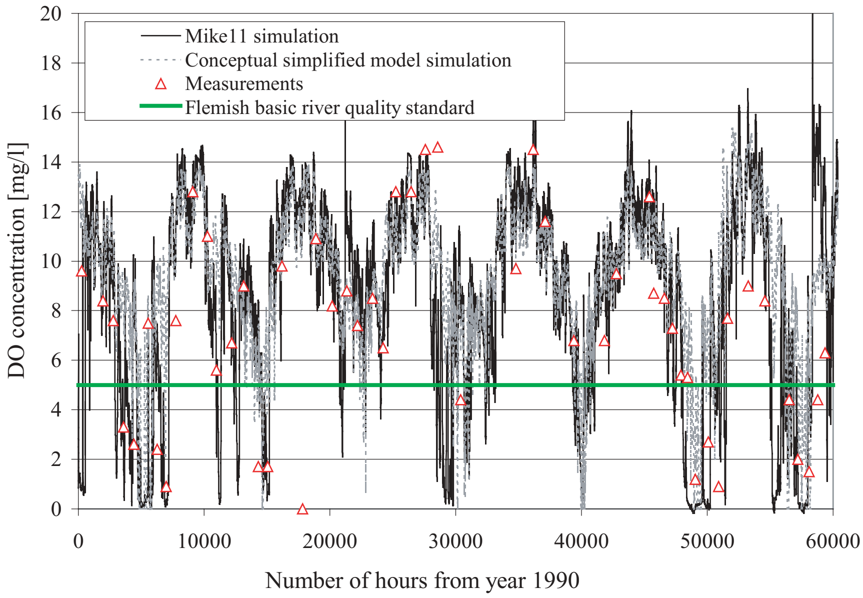


Figure 6 Modelled DO concentrations for both models against the observed data.

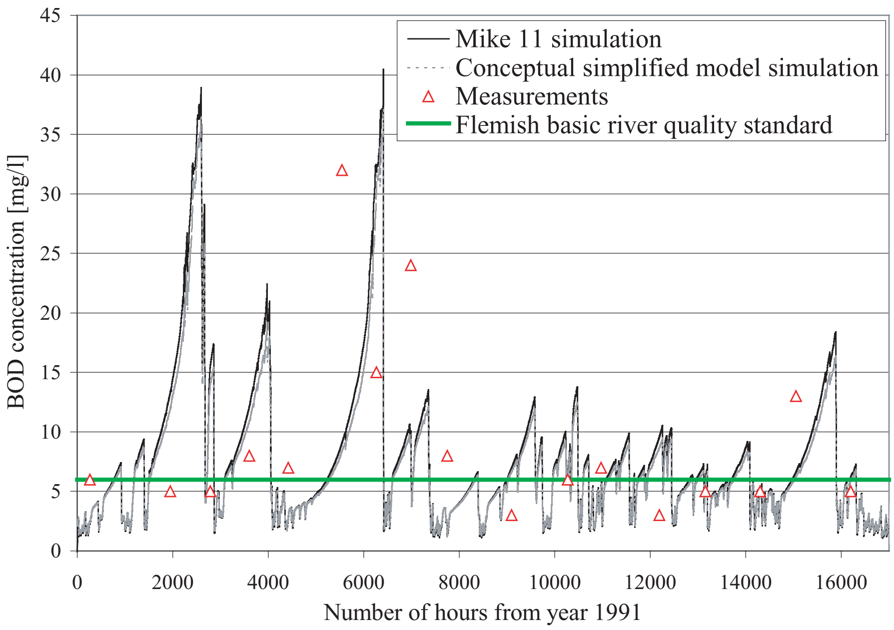


Figure 7 Modelled BOD concentrations for both models against the observed data.

A more detailed analysis of these uncertainty sources and its contribution to the total uncertainty in the model results can be found in Radwan *et al.* (2003).

Based on both the modelled and the observed concentrations, it is concluded that the standards are not met for BOD. This problem is mainly encountered in summer time as a consequence of the combination of low river discharges and pollutant loads. During the periods with high river discharges, the water quality in the river indeed meets the standards. The comparison of the two models shows that the conceptual simplified model behaves almost the same as the detailed Mike11 model.

Two aspects of adequacy of model results are highlighted, namely accuracy and model speed. Model accuracy is defined as the difference between the modelled and observed values. Model speed is considered very important to be able to perform long-term simulations and to analyse the river water quality state in a statistical way. It is also important if one wants to perform an uncertainty analysis. Indeed, in such analysis, many computer runs are needed. According to the speed, the conceptual simplified model is much faster than the Mike11 model. To run a 1-year simulation with the Mike11 model, 1 hour is needed, but with the conceptual simplified model, only 2 seconds are needed. The conceptual simplified model is 1800 times faster. The accuracy of the two models is measured as the difference between the simulated values and the reality. This study could not be done very accurately, because the mean measurement frequency is only approximately 1 per month. The standard deviation of the residuals between the measurements and the average simulated values of the same measurement day is calculated. The results are presented in Table 1. It is concluded that the two models have similar accuracy.

Also an extreme value analysis is conducted for the simulation results of both models. In the detailed Mike11 model, a time series of 8 years was simulated and the results compared with the simulation in the conceptual simplified model (after excluding the 1st year of the simulation because of the influence of the initial conditions in the model). The result for BOD is presented in Figure 8. It shows that the extremes of the two models almost behave in the same way.

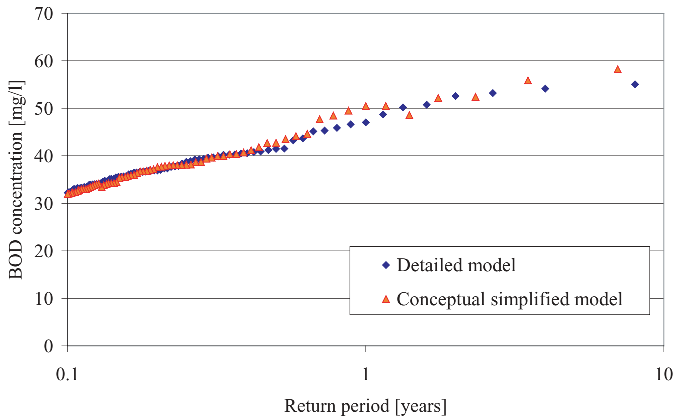


Figure 8 Comparison of the modelled extreme value distribution of BOD concentration for both the detailed and the conceptual simplified models.

## Conclusion

Different model types are available to model catchment surface water quality. They vary from detailed physically-based models to simplified conceptual and empirical models. The most appropriate model type for a certain application depends on the project objectives and the data availability. Organic domestic sources and nitrogen sources (agricultural leaching and domestic point sources) were considered as input to the model. Based on these sources, concentrations of DO and BOD were modelled by two models with different level of complexities. The calibration was done on the basis of available measured water quality data. A more simplified model was calibrated to the detailed model with the objective to yield much faster long-term simulation results which can be used in a statistical analysis. Two aspects of adequacy of model results are highlighted, namely accuracy and model speed. The conceptual simplified model is 1800 times faster than the detailed Mike11 model. Moreover, the two models have almost the same accuracy. Therefore, the conceptual simplified model is recommended for long-term simulations as it includes only the most important and sensitive processes, but must be calibrated against results from the detailed model. In addition, as less input data is needed to run the simplified model, it is expected that the total uncertainty of the results is smaller. The non-sensitive processes indeed most often require additional input variables, with input uncertainties associated to these variables. These input variables and uncertainties are excluded from the simplified model.

Finally, the detailed models are recommended for short-term simulations with parameters calibrated to the observed data. This calibration can only be done in an accurate way when sufficient data is available for model input and model parameters. The detailed model is also needed to calibrate the simplified model (the parameters of the conceptual representation of the advection and dispersion processes), and to identify the most sensitive water quality processes. Water quality data is in most cases still insufficient to have a direct calibration of conceptual simplified models. More detailed physically-based models are needed to be used in combination with the limited data available. This also means that the simplified model has to be recalibrated each time local conditions change significantly (e.g. when different water management scenario's are considered), or when the model is applied to another river. More details about this work can be found in Radwan (2002).

Table 1 Comparison of the standard deviation for both the Mike11 and the conceptual simplified model.

| Modelled parameter | The standard deviation | |
|---|---|---|
| | Mike11 | Conceptual simplified model |
| DO | 1.49 | 1.38 |
| BOD | 1.16 | 1.11 |

**Acknowledgements**

The water quality data of the Molenbeek brook has been made available by the Flemish Environmental Agency (VMM). Data for the hydrodynamic river model has been provided by the Flemish Water Authority AMINAL and the consultant agency IMDC.

The work is supported by the Fund for Scientific Research – Flanders (F.W.O. – Vlaanderen), through the postdoctoral scholarship of P. Willems.

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