UNIVERSITEIT GENT

FACULTEIT LANDBOUWKUNDIGE EN
TOEGEPASTE BIOLOGISCHE
WETENSCHAPPEN

Academiejaar 2003-2004

DYNAMIC INTEGRATED MODELLING OF BASIC WATER QUALITY AND FATE AND EFFECT OF ORGANIC CONTAMINANTS IN RIVERS

GEINTEGREERDE DYNAMISCHE MODELLERING VAN ALGEMENE WATERKWALITEITSPARAMETERS EN GEDRAG EN EFFECT VAN ORGANISCHE CONTAMINANTEN IN RIVIEREN

door

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Thesis submitted in fulfillment of the requirements for the degree of Doctor (Ph.D.) in Applied Biological Sciences: Environmental Technology

Proefschrift voorgedragen tot het bekomen van de graad van Doctor in de Toegepaste Biologische Wetenschappen: Milieutechnologie

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Summary

Both conventional pollutants and organic contaminants in rivers are of concern to the water quality managers and environmental risk regulators to achieve water quality objectives. After an extensive literature study made in Chapter 2 it becomes clear that the complexity of ecological problems (particularly the interaction between conventional pollutants and organic contaminants) requires a different approach than traditional river water quality models can provide. The traditional models are focusing on the two issues separately, and hence, do not consider the interaction between the two main water quality problems. They also lack appropriate linking processes and state variables, and, thus, they cannot be coupled without modification.

The ultimate goal of this work is to develop a dynamic integrated model of conventional pollutants and organic contaminant fate and effect in rivers. This integrated modelling approach is a holistic approach that assists the water quality managers and environmental risk regulators to achieve a "good" biological water quality.

In this work, three key problems are addressed in order to achieve this goal (dynamic integrated river water quality modelling). The first problem is related to the complexity of the hydrodynamic model (the St. Venant equations) and the basic water quality model that is typically used to describe river water quality under unsteady state conditions. As the St. Venant equations require a long computation time, extending these equations for dynamic integrated modelling of basic water quality and organic contaminant fate and effect is not practically feasible. For instance, the River Water Quality Model No. 1 (RWQM1) is the most comprehensive basic river water quality model available in literature. It is, however, too complex to be applied in data limited situations, especially in developing countries.

The second problem is related to the development of a realistic organic contaminant fate (exposure) model. The current methods of risk assessment or regulation are based on steady state models (fugacity level III), e.g. in the EU member countries. However, as environmental conditions are never at steady state, this steady state model cannot be readily validated. Besides, such a modelling approach lacks appropriate process descriptions and state variables, and, hence, cannot describe observed short-term dynamics of organic contaminants in rivers.

The third problem is that traditional river water quality modelling describes both conventional pollutants and organic contaminants as separate issues. The effect of nutrient dynamics on the fate of organic contaminants and vice versa is not taken into account.

In this Ph.D. thesis, an attempt was made to tackle these three problems in four steps. First, a conceptual hydraulic model (Continuously Stirred Tank Reactors in Series) was applied as a surrogate to a complex hydrodynamic model. This conceptual approach applies only to rivers where tidal (or backwater) effects are absent. The optimum number of tanks-in-series required for this concept is best determined on the basis of a tracer study.

Second, the RWQM1 was simplified so that the model can be applied in data limited situations. The application of the simplified model was evaluated using a case study of inorganic nitrogen and total dissolved solids in the Crocodile River (South Africa). The results of model calibration and validation indicate that the proposed model can adequately describe the seasonal dynamics of inorganic nitrogen in that river. Two water quality management options were also investigated in order to improve the downstream water quality of the Crocodile River: (1) setting a maximum upstream freshwater withdrawal and (2) applying low flow augmentation. The results show that

despite the fact that both methods can improve the downstream river water quality, a stringent urban water pollution prevention plan is also needed.

Third, a dynamic in-stream fate (exposure) model was developed on the basis of the conceptual hydraulic model and the simplified RWQM1. The simplified RWQM1 was extended in order to include a xenobiotic organic contaminant fate submodel. The usefulness of the proposed organic contaminant fate model was investigated using a Linear Alkylbenzene Sulphonate (LAS) case study in the River Lambro (Italy). The results indicate that the proposed model can adequately describe the short-term dynamics of LAS in the River Lambro. The effect of conventional pollutants (nutrients) on the in-stream fate of LAS was also investigated using an artificial river, and the in-stream fate model was further refined based on the results of the artificial river study. The proposed dynamic exposure model can simulate the time evolution of the exposure concentration in three phases of environmental compartments (water and benthic sediment): truly dissolved, sorbed to dissolved organic carbon and suspended solids in the bulk water; truly dissolved and sorbed to dissolved organic carbon in the pore water, and sorbed to benthic sediment. These different concentrations of contaminants in the three phases are needed to allow the proposed exposure model to be linked to the bioaccumulation and toxicokinetic submodels. Subsequently, dynamic effect/toxicity can be simulated, with the latter submodels.

Fourth, by linking the basic water quality submodel (for conventional pollutants) to the proposed organic contaminant fate and effect submodels, a dynamic integrated river water quality model was developed. Linking individual submodels was done by selecting appropriate linking processes or linking variables. The linking processes are part of the carbon cycle, whereas the linking variables are microbial biomass, particulate organic carbon, dissolved organic carbon, dissolved oxygen and mineral nutrients. The proposed model describes not only the time evolution of conventional pollutants and organic contaminants in rivers, but also the interaction between eutrophication and contamination by xenobiotic organic compounds. The model can, hence, simulate the effect of conventional pollutants on the fate and effect/toxicity of organic contaminants in rivers. The usefulness of the model was evaluated using a case study of LAS in the river Lambro with some scenario analyses such as the effect of nutrients and total suspended solids, the partition coefficient and the contamination frequency of the river by Combined Sewer Overflows (CSOs). The results of model validation and scenario analyses show that the model can adequately describe fate and effect of LAS in the river Lambro. A higher exposure frequency can increase toxicity, which depends on the critical body burden. The trends show that on increase of ammonia nitrogen concentration in an oligotrophic river system can decrease the predicted LAS tissue concentration.

Summarizing, this work has introduced some important new concepts, e.g. modelling dynamic exposure and the interaction of conventional pollutants and organic contaminants in rivers. It as such addresses important issues for water resource management. Much work, however, still needs to be done in the framework of integrated ecological risk assessment and integrated water quality management: extending the proposed concepts for other important hazardous substances; considering mixture toxicity and multiple stressors; appropriate ecological modelling for dynamic effect assessment; and considering the uncertainty associated with those most sensitive model inputs.