

ADVECTION-DISPERSION MODEL FOR NUTRIENT DYNAMICS IN RIVER SWALE

Elisabeta C. Ani^{*}, Michael G. Hutchins[†] and Paul S. Agachi^{*}

^{*} Faculty of Chemistry and Chemical Engineering, "Babes-Bolyai" University Cluj-Napoca
11, Arany Janos Street, 400028, Cluj-Napoca, Cluj, Romania
E-mail: eani@chem.ubbcluj.ro; sagachi@chem.ubbcluj.ro, web page: www.chem.ubbcluj.ro

[†] Centre for Ecology and Hydrology Wallingford
Maclean Building, Crowmarsh Gifford, Wallingford, Oxfordshire, OX10 8BB, England, UK
E-mail: mihu@ceh.ac.uk; web page: www.ceh.ac.uk

Key words: pollutant transport modelling, ADMModel, water quality model, phosphorus, nitrogen, and River Swale.

Summary. *This paper presents a detailed mathematical model (ADMModel) for the transport of nutrients (nitrate; ammonium; soluble reactive phosphorus and organic phosphorus) under unsteady flow conditions in River Swale.*

1 INTRODUCTION

River Swale drains a basin of approximately 1350 km² in North England. The present paper is focused on the mathematical modelling of nutrient transport along a short stretch (50.4km). Investigated nutrients (nitrate (NO₃), ammonium (NH₄), soluble reactive phosphorus (SRP) and organic phosphorus (OP)) play a major role for the water quality of River Swale.^{5,6,9} These nitrogen and phosphorus compounds are very common pollutants of running waters, and especially of rivers crossing inhabited areas or agricultural fields, due to anthropogenic pressure. They are critical nutrients limiting the quality of river water, being vital for the development of biological organisms and also damaging via eutrophication.⁵

River Swale was subjected to a large number of water quality research studies, the most significant being LOIS, a major UK environmental research initiative including the development of modelling software (QUESTOR^{4,8}). QUESTOR applications in LOIS addressed the Swale within modelling of the larger Ouse catchment (approx. 3500 km²). In LOIS very little research has been directed to detailed study of short river stretches. Rather than for the detailed modelling studies of short river stretches (e.g. plume dispersion studies, pollutant transport after accidental release), QUESTOR is suitable for the modelling of large rivers at daily time resolution.⁷ Swale is also the subject of several studies focused on the estimation of nutrient dynamics,^{6,5,9} but they are not focused on the prediction of pollutant transport along the river.

In the present research the analytical solution of the fundamental advection-dispersion equation (ADE) for mass transport in rivers was used to develop a detailed mathematical model for nutrient transport in River Swale (ADMModel).

These kind of advection-dispersion analytical models have as main advantages the quality of results, the short computation time they need, lower computation resources compared to numerical model and user-friendly post processing of results. Possible disadvantages of such analytical model are related to: (1) the representation of hydraulic non-uniformity of the river stretch; and (2) the inclusion of influences (tributaries, pollution sources, abstractions). To attend these issues the river stretch is divided in reaches, each one having a constant average value of hydraulic parameters and including influences at the beginning of reach.^{7,8} This approach complicates the applicability of the model to other rivers, and has been replaced in the present research by a more useful method explained elsewhere (Ani et al., 2009b).

ADModel offers a different and more detailed perspective of studying pollutant transport compared to many existing studies and models (e.g. QUESTOR). Existing approaches are typically based on a broad characterisation of chemical status and how it varies within large river basins. These existing models (1) represent the river as a perfect mixed tank or as a succession of perfect mixed reaches; (2) assume constant average parameters of the river/reaches; (3) make predictions at large time steps (daily); and (4) locate pollution sources and abstractions at reaches boundaries; while ADModel (1) represents the river as a continuous computational domain; (2) with variable parameters along it; (3) predicts concentration at smaller time steps (hourly); and (4) locate pollution sources and abstractions at the real place along the river.

This enables ADModel to be useful to predict the propagation of the four investigated nutrients at any place along the river stretch (under normal and accidental discharge) while existing models predict pollutant dynamics just at reach boundaries. Study and explanation of nutrient dynamics in the river stretch in terms of the temporal variability of the nutrient transformation rates is also possible.

2 MODEL DEVELOPMENT

ADModel is based on the analytical solutions (2)^{3,14} (plus a module for pollutant transformations) of ADE (1)^{3,14}. More details on the convective-diffusive transport in rivers, on ADE and its analytical solutions are provided elsewhere.¹⁴

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right) - \frac{\partial(cV)}{\partial x} \pm kc \quad (1)$$

$$c(x, t) = c_0 + \frac{(c_s - c_0)}{2} \left[\operatorname{erfc} \left(\frac{x - Vt}{\sqrt{4Dt}} \right) + \exp \left(-\frac{xV}{D} \right) \operatorname{erfc} \left(\frac{x + Vt}{\sqrt{4Dt}} \right) \right] \quad (2)$$

where c [mg/L] is the pollutant concentration in time (t [s]) along the river length (x [m]); D [m^2/s] is the longitudinal dispersion coefficient; V [m/s] is the convective velocity; k [1/s] gives the pollutant transformations through first order kinetics; c_0 [mg/L] is the initial concentration along the river stretch (x [m]), assuming nonzero initial condition throughout the river; and c_s [mg/L] is the concentration at source.

A short description of the ADModel taking into account some important features is listed in Table 1. A part of these features correspond to criteria according to which pollutant transport models can be classified (e.g. type of solution employed for ADE; release duration; representation of transformations).

Model	ADModel for River Swale
Implementation	ADE analytical solution implemented in Matlab
Pollutant release	Four continuous pollution sources Three tributaries
Abstractions	15
Pollutants	NH ₄ , NO ₃ , SRP, OP
Transformations	Nitrification, denitrification, mineralization
Transformation rates	QUESTOR calibrated values
Parameter models	Velocity; Dispersion coefficient
Water flow	Unsteady
Inputs concentration and water flow	Pollution sources: constant Tributaries: unsteady
Other features	Pollutant transport under normal and accidental discharge can be simulated. More sources, discharging along the river stretch, could be implemented.

Table 1: Main features of ADModel.

The model development, calibration and validation rely on experimental data obtained during ten monitoring campaigns carried out with the river in low and medium flow, but also under storm conditions. Monitoring of concentration, water flow and water depth, was done at up to four sites (further referred to as M1 to M4) along the river stretch. These variables are used in the model as time series. Measurements of river channel parameters (water depth, channel width, river bed slope) are also available. Detailed information on: campaigns, monitoring sites, monitored parameters; are published elsewhere.³

The ambitious task during the development of ADModel was (i) to take into account the dynamic of river hydraulic parameters and (ii) to include in the analytical model multiple pollution sources characterised by time series of changing flow and concentration. These features, along with the number of pollutants and their transformations, increase the model complexity.

The analytical solution of ADE, along with equations for the parameters was implemented in Matlab. Parameters characterizing the nutrient transport along the river are implemented in the model as explained below.

- Velocity and longitudinal dispersion coefficient were first calculated using experimental data and optimized during calibration. Using optimum values models for their estimation as functions of the hydraulic parameters were established.³

- Transformation rates use QUESTOR underlying equations, calibrated for the river stretch of interest.^{3,8} They capture the influence of temperature and/or unsteady water flow on the constants controlling transformation rates.

The present research overcomes problems related to channel hydraulic non-uniformity and inclusion of influences by using a single river reach, parameterized according to the novel approach proposed by Ani et al. (2009b). The method (A) enables pollution sources, tributaries and abstractions to be positioned in the model at the real distance along the main channel and not at the beginning of reaches; (B) makes ADModel capable to predict the propagation of the four nutrients at any place along the river stretch, while existing models predict pollutant dynamics just at reach boundaries; and (C) enables the study and explanation of nutrient dynamics in the river stretch in terms of the temporal variability of the nutrient transformation rates.

Another interesting feature of ADModel, compared to most of the existing analytical models^{13,10} is the possibility to consider the water flow change in time, not just in space along the river. In this way the model parameters depending on water flow are described as changing in time as well; tributaries are characterised by unsteady pollutant concentration and discharge; and pollution sources also.

3 SIMULATION RESULTS AND DISCUSSION

ADModel was applied to data from wide ranging water flow conditions: from a minima of 2.45 m³/s to a maxima of 196.79 m³/s. ADModel was set to behave as: (a) conservative model, with transformation rates set to zero; and (b) non-conservative model, using QUESTOR calibrated transformation rates.

Model results for a low flow monitoring campaign (#3, 27-31 October 1995) and a high flow monitoring campaign (#4, 22-26 February 1996) are shown below for exemplification purposes. Water flow is increasing from M1 to M4 and for each site systematically decreasing in time (e.g. Figure 1 and Figure 2).

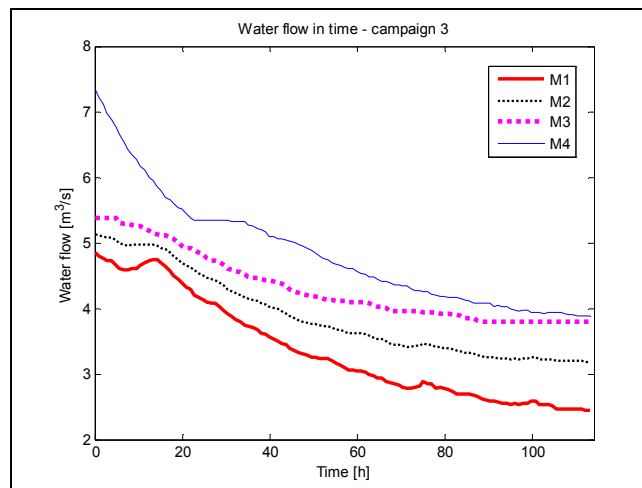


Figure 1 Water flow in time at monitoring sites M1 to M4 during campaign 3 (low flow)

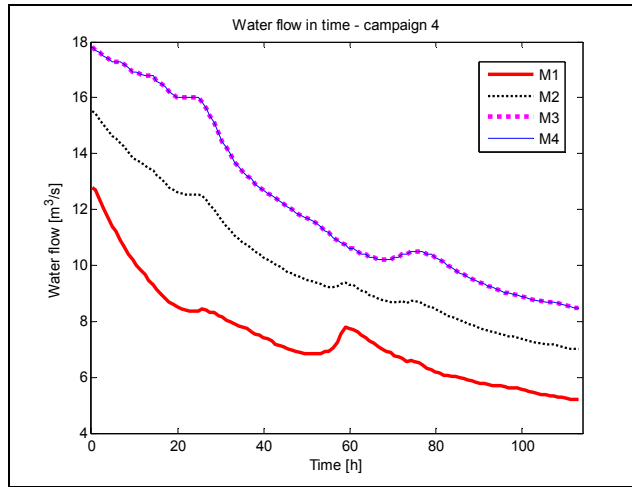


Figure 2 Water flow in time at monitoring sites M1 to M4 during campaign 4 (high flow)

During almost all campaigns large differences between water flow values can be observed between the first three monitoring sites; while very small differences are observed between M3 and M4. This is due to the location of major tributaries and pollution sources (e.g. sewage treatment works, quarry) upstream M3. Tributaries and pollution sources also discharge nitrogen and phosphorus compounds into the main channel, contributing to the increase of pollutant concentration along the stretch (Kim et al., 2006; Bowes and House, 2001; House et al., 1997). Differences between monitored concentration of each species at M1 and M4 are shown in Figure 3 to Figure 6.

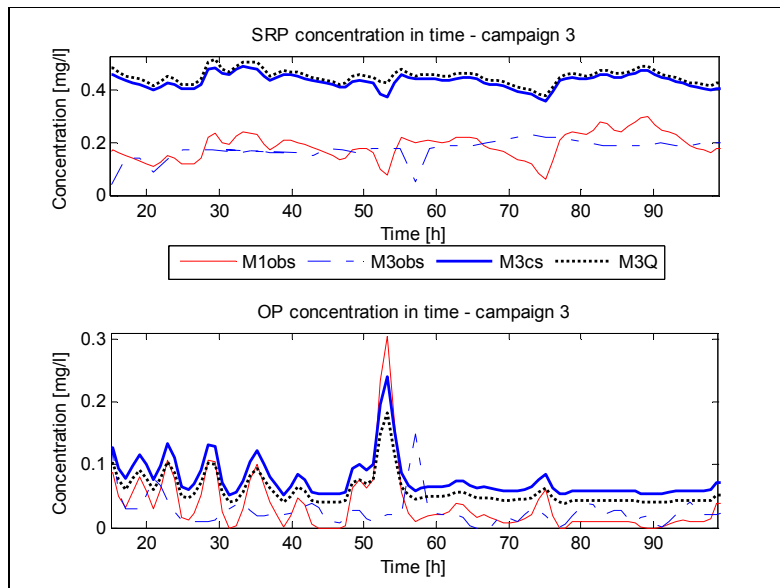


Figure 3 SRP and OP concentration during campaign 7 (low flow)

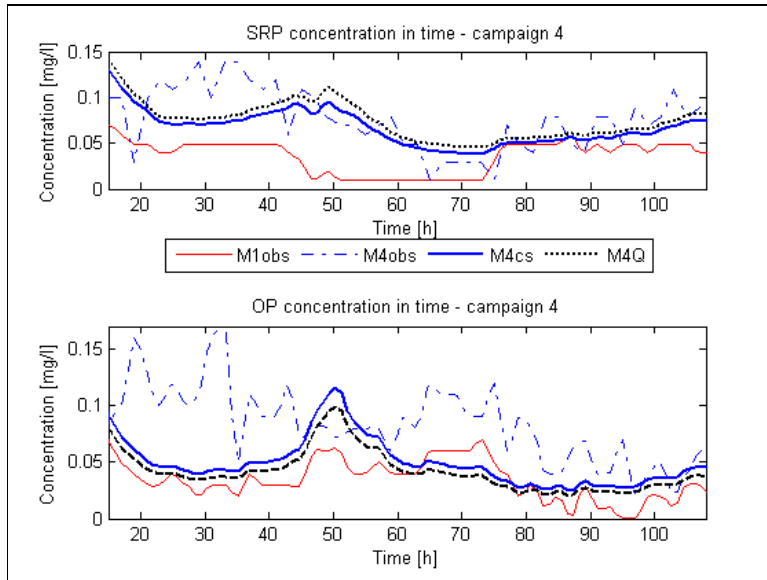


Figure 4 SRP and OP concentration during campaign 4 (high flow)

Pollutant concentration at M1, along with concentration discharged by pollution sources and tributaries is used as input for ADModel. The expected output is the evolution of pollutant concentration at downstream monitoring sites. ADModel proved to be capable to predict the main trend of measured concentration at these sites and to account for changes in water flow and pollutant load in time between sites.

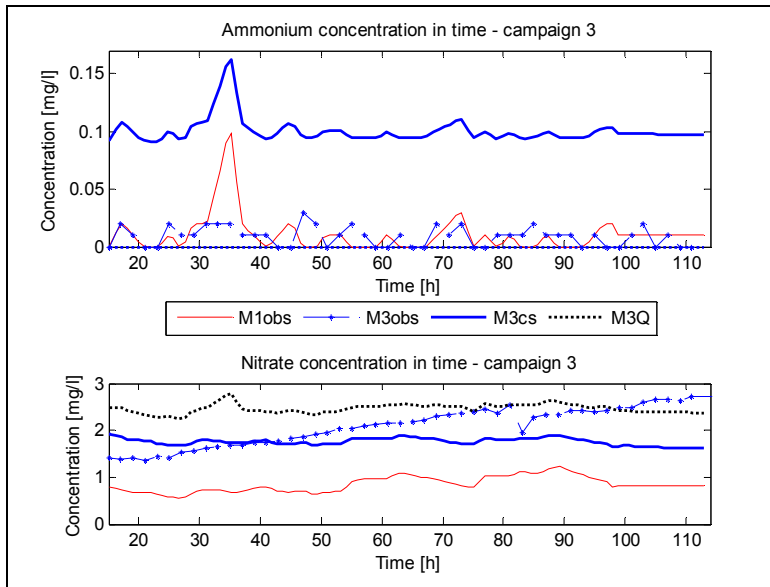


Figure 5 Nitrate and ammonium concentration during campaign 3 (low flow)

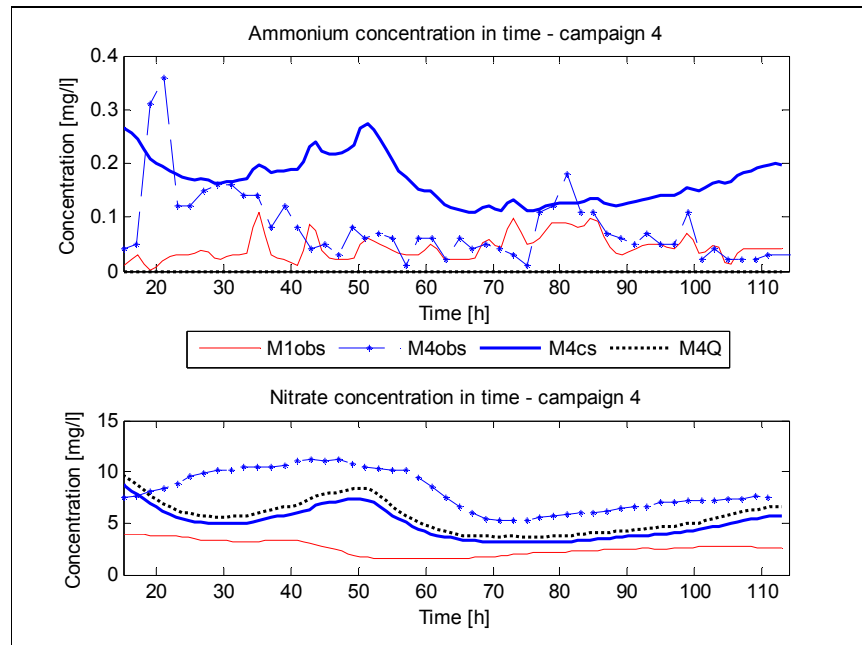


Figure 6 Nitrate and ammonium concentration during campaign 4 (high flow)

In the most of runs ADMModel using QUESTOR transformation rates lead to better prediction of nutrient concentration compared to conservative ADMModel. This shows that nutrient transformations play a key role during nutrient transport along Swale (see Figure 3 to Figure 6). Generally phosphorus compounds are predicted better compared to nitrogen compounds.

At low flows OP is given better predictions than SRP, and at medium and high flows (campaigns #1, 4, 8, 9 and 10) SRP concentration is given better prediction than OP. Prediction could be improved by including in ADMModel the sedimentation and re-suspension of OP, in order to correlate its variability with water flow: additional OP consumption will take place trough sedimentation at low flows, while additional OP gain will be done trough re-suspension especially at high flows.

The conservative ADMModel predicts nitrate better than ammonium, while non-conservative ADMModel predicts ammonium better. This is because ammonium is more sensitive to transformation (nitrification) compared to nitrate (nitrification and denitrification). Nitrification takes place all times, while denitrification takes place mostly at low flows.

ADMModel is useful for water quality policy makers, for managers and also for researchers. For policy makers and managers it is useful to assess the effects of pollution sources on river water quality, as it is possible to estimate the river distance affected by pollutant release, the duration of release effects, and the magnitude of problems. The model enables the study of technological improvements (e.g. changes to effluent treatment systems) or investigations related to development of new facilities (e.g. industrial sites, houses, livestock farms). The study of environmental effects of these modifications is important as they affect water quality

of rivers. Parameters interdependence (e.g. water flow, transformation rates, dispersion coefficient) and their influence on pollutant transport could also be investigated using pollutant transport models. From this perspective ADModel is very useful for the research sector.

4 CONCLUSIONS

The present paper concerns nutrient transport modelling at small time steps (one hour), using analytical solutions of ADE, not employed previously in a similar way for River Swale. Developed model is useful for the prediction of pollutant concentration in case of usual and/or accidental chemicals release, from both continuous sources, under unsteady water flow. ADModel proved to be capable to predict the main trend of measured concentration during a wide range of water flows and to account for changes in pollutant load in time between sites. Simulation results show the importance of transformation processes during nutrient transport in River Swale.

REFERENCES

- 1 E.C. Ani, *Minimization of the experimental workload for the prediction of pollutants propagation in rivers. Mathematical modelling and knowledge re-use*. Acta Universitatis Lappeenrantaensis 355, Lappeenranta teknillinen yliopisto, Digipaino, Lappeenranta, Finland, pp. 189, (2009).
- 2 E.C. Ani, S.G. Wallis, A. Kraslawski, P.S. Agachi, "Detailed mathematical model for pollutants transport in a natural stream", *Computer Aided Chemical Engineering*, **26**, 731-736, (2009b).
- 3 E.C. Ani, M.G. Hutchins, A. Kraslawski, P.S. Agachi, "Mathematical model to identify nitrogen variability in large rivers", *River Res Appl*, in press (2010).
- 4 D.B. Boorman, "LOIS in-stream water quality modelling. Part 1. Catchments and methods", *Sci Total Environ*, **314-316**, 379-395, (2003).
- 5 M.J. Bowes, W.A. House, R.A. Hodgkinson, "Phosphorus dynamics along a river continuum", *Sci Total Environ*, **313**, 199-212, (2003).
- 6 M.J. Bowes and W.A. House, "Phosphorus and dissolved silicon dynamics in the River Swale catchment, UK: a mass-balance approach", *Hydroll Process*, **15**, 261-280, (2001).
- 7 A. Deflandre, R.J. Williams, F.J. Elorza, J. Mira, D.B. Boorman, "Analysis of the QUESTOR water quality model using a Fourier amplitude sensitivity test (FAST) for two UK Rivers", *Sci Total Environ*, **360**, 290-304, (2006).
- 8 A. Eatherall, D.B. Boorman, R.J. Williams, R. Kowe, "Modelling in-stream water quality in LOIS", *Sci Total Environ*, **210/211**, 499-517, (1998).
- 9 W.A. House and M.S. Warwick, "A mass-balance approach to quantify the importance of in-stream processes during nutrient transport in a large river catchment", *Sci Total Environ*, **210/211**, 111-137, (1998).
- 10 W.A. House, D. Leach, M.S. Warwick, M.S. Whitton, S.N. Pattinson, G. Ryland, A. Pinder, J. Ingram, J.P. Lishman, S.M. Smith, E. Rigg, F.H. Denison, "Nutrient transport

- in the Humber rivers”, *Sci Total Environ.* **194/195**, 303-320, (1997).
- 11 K. Kim, P. Kalita, M.J. Bowes, J.W. Eheart, “Modeling of river dynamics of phosphorus under unsteady flow conditions”, *Water Resour. Res.* **42**, **7**, W07413, doi:10.1029/2005WR004210, (2006).
 - 12 R.L. Runkel and K.E. Bencala, “Transport of reacting solutes in rivers and streams”. In: Singh, V.P. (Ed.). *Environmental Hydrology*. The Netherlands, Kluwer Academic Publishers, 137-164, (1995).
 - 13 A. Sanchez-Cabeza and L. Pujol, “Study on the hydrodynamics of the Ebro river lower course using tritium as a radiotracer”, *Wat Res*, **33**, 10, 2345-2356, (1999).
 - 14 S.A. Socolofsky and G.H. Jirka, *Special Topics in Mixing and Transport Processes in the Environment*. Engineering – Lectures. 5th Edition. Coastal and Ocean Engineering Division. Texas A&M University, (2005).