DYNAMIC EXPOSURE ASSESSMENT AND MODELLING

Tolessa Deksissa[1], Peter A. Vanrolleghem[1]

[1]Ghent University - BIOMATH, Department of Applied Mathematics, Biometrics and Process Control, Coupure Links 653, B-9000 Gent, BELGIUM

Objectives

Risk assessment requires the comparison of Predicted Environmental Concentration (PEC) and Predicted No Effect Concentration (PNEC). The current PEC estimation method in the European union is based on a steady state in-steam fate model [1]. This model assumes uniform flow emissions, and does not consider temporal variability in the system.

Thus, the Objectives of this study include:

- To develop a short time dynamic environmental fate model for rivers, and
- To evaluate this model in view of dynamic exposure assessment.

Model

- Linear Alkylbenzenesulfonates (LAS), an anionic surfactant, is subject to different physicochemical and biological decay processes in rivers (Fig. 2).
- Considering only the dominant processes, and using a completely mixed tank in series model, the mass balance in every river tank for the dissolved phase can be expressed as:

$$\frac{d(CV)}{dt} = Q_{in}C_{in} - Q_{out}C - k_{elm}CV \quad (1)$$

$$k_{elm} = \frac{1}{(1+K_P r_P + K_{doc} r_{doc})} \cdot \begin{pmatrix} (k_s + k_{biodeg})K_P r_P + k_{biodeg} \\ + k_V + k_{biodeg} K_{doc} r_{doc} \\ + K_P \frac{dr_P}{dt} + K_{doc} \frac{dr_{doc}}{dt} \end{pmatrix}$$

Where V = the volume of the tank [m^3],

Q_{in} & Q_{out} = the inflow rate and outflow rate respectively [$m^3 d^{-1}$],

C_{in} & C = the inflow and outflow concentration respectively [mgL^{-1}],

k_{elm} = the overall pseudo first order in-stream elimination rate constant [d^{-1}],

k_s = pseudo first order rate constant for the net sedimentation [d^{-1}]

k_V = pseudo first order rate constant for volatilization [d^{-1}]

k_{biodeg} = pseudo first order rate constant for biodegradation [d^{-1}]

$?_{doc}$ = the Dissolved Organic Carbon density/concentration (DOC) [mg L^{-1}],

$?_p$ = suspended particulate density/concentration [mg L^{-1}],

K_P = the particulates-water partition coefficient [L mg^{-1}], and

K_{doc} = the DOC-water partition coefficient [L mg^{-1}].

Assumptions:

- Local equilibrium between sorbed and dissolved ($C_{total} = C_{dissolved} + C_{sorbed}$)
- Equal degradation rate for both sorption and desorption
- LAS biodegradation carried out only in aerobic conditions
- No atmospheric deposition
- Chemical removal due to hydrolysis, photolysis, bioaccumulation, and sediment burial are negligible

Case Study

- The river stretch of 26 km (part of river Lambro, in Italy) between Mulino de Baggero and Biassono) divided into 4 monitoring stations that are further subdivided into in total 47 completely mixed tank in series [2].
- LAS pollution sources: treated (wastewater treatment plant ,WWTP, effluent) and untreated (combined sewer over flows, CSO) wastewater with variable flow emissions.

Figure 1. Map of the study site, the river Lambro

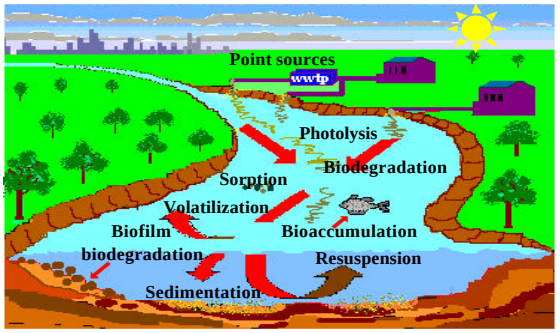

Figure 2. General representation of in-stream fate of toxic organic chemicals

Results

- Using the WEST® modelling and simulation software (Hemmis NV, Kortrijk, Belgium), and the monitoring data of February 1998 [3], the simulation results illustrated in Figure 3 and Table 1 are obtained.

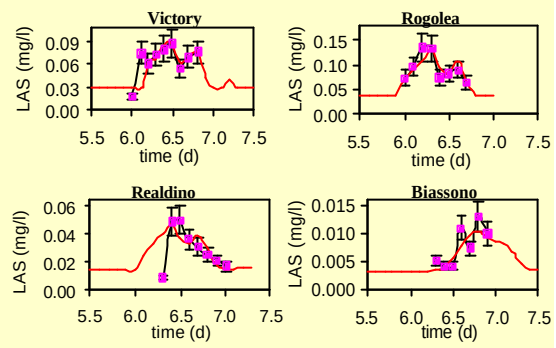

Figure 3. Comparison of measured (ϖ) and simulated (–) data set in four river sections

Table 1. Comparison of average measured and simulated data sets

River section	Distance (km)	Measured LAS (mg/l)	Simulated LAS (mg/l)
Rogolea	1.5	0.088	0.086
Victory	6.3	0.061	0.062
Realdino	15.6	0.030	0.028
Biassono	25.9	0.007	0.007

Discussion

- The general trend of simulated data sets agrees well with the measured data within 20% error (Figure 3).
- The average predicted data sets are almost equal to the average measured data sets in every river section (Table 1).
- Of the overall LAS in-stream removal, 71.5% is due to biodegradation and 28,5% is due to sorption to suspended particulates.
- The contribution of volatilization and sorption to DOC is negligible because LAS has a very low vapor pressure and hydrophilic nature respectively.

TAKE HOME MESSAGE

- Dynamic exposure model is a realistic approach for time variable emissions.
- A multi-compartment (air, water and sediment phases) model is more realistic than using just one compartment model for exposure assessment.

Acknowledgement

- The authors thank the Belgium Technical Co-operation (BTC-CTB) for its financial support, and members of the GREAT-ER ECETOC task force for the supply of data.

References

[1] OECD (1999). Environmental exposure assessment for existing industrial chemical in OECD member countries. Series of testing and assessment No. 17.

[2] Meirlaen, J., Huyghebaert, B., Sforzi, F., Benedetti, L. and Vanrolleghem, P.A. (2001). Simultaneous simulation of the integrated urban wastewater system using mechanistic surrogate models. *Wat. Sci. Tech.* **43** (7) 301-309.

[3] Whelan, M .J., Gandolfi, C. and Bischetti, G.B. (1999). A simple stochastic model of point source solute transport in rivers based on gauging station data with implications for sampling requirements. *Water Res.* **33** (14) 3171–3181.

BIOMATH tolessa@biomath.rug.ac.be - http://biomath.rug.ac.be