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## INTRODUCTION

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-stream fate model [1]. This model assumes uniform flow emissions, and does not consider temporal variability in the system. However, dynamic exposure assessment accounts for the temporal variability.

Thus, the objectives of this study are:

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

## MODEL FORMULATION

- Linear Alkylbenzenesulfonates (LAS), an anionic surfactant, is toxic and can be subjected to different physicochemical and biological decay processes in rivers (see Figure 1).
- Using a completely mixed tank in series model, the mass balance for the total LAS in the water phase in every river tank can be expressed as follows:

$$\frac{d(C_T V)}{dt} = Q_{in} C_{T,in} - Q_e C_T - k_{rem} C_T V + S_{external}$$

$$k_{rem} = k_{bio\ deg} + k_{sed} + k_{vol}$$

Where  $V$  is the volume of the tank [m<sup>3</sup>],  $Q_{in}$  &  $Q_e$  are respectively the inflow rate and outflow rate [m<sup>3</sup>d<sup>-1</sup>];  $C_{T,in}$  &  $C_T$  are concentrations in the inflow and outflow, respectively [g m<sup>-3</sup>];  $k_{rem}$ ,  $k_{sed}$ ,  $k_{bio\ deg}$  and  $k_{vol}$  are the overall pseudo first order in-stream removal, sedimentation, biodegradation and volatilization rate constants, respectively [d<sup>-1</sup>];  $S_{external}$  is the external source due to resuspension [g d<sup>-1</sup>].

### Assumptions:

- Local equilibrium between sorbed and dissolved ( $C_{total} = C_{dissolved} + C_{sorbed}$ ).
- Equal degradation rate for both sorbed (in the Dissolved Organic Carbon (DOC) and Particulated Organic Carbon (POC)) and dissolved phases.
- Aerobic biodegradation in the bulk water and in the benthic sediment (biofilm).
- Atmospheric deposition, photolysis, bioaccumulation and sediment burial are negligible.

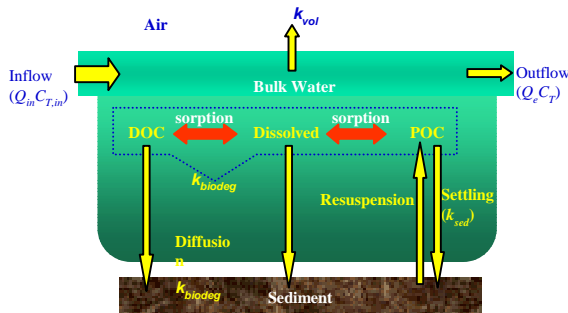


Figure 1. General representation of in-stream fate of toxic organic chemicals

## CASE STUDY

- LAS pollution sources: treated (wastewater treatment plant effluent) and untreated combined sewer overflows wastewater with variable flow emissions.
- The river stretch of 26 km (part of river Lambro, in Italy) between Mulino di Baggero and Biassono) was divided into 4 monitoring stations (see Figure 2) that were subdivided into the total 11 completely mixed tanks in series (see Figure 3). Each tank was further subdivided (1- 6), and in total 47 tanks were used [2].

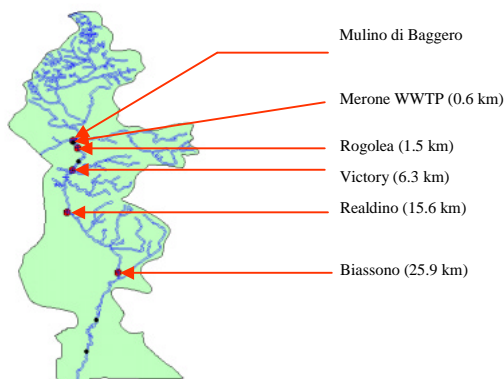


Figure 2. Scheme of river Lambro with four monitoring stations

## RESULTS AND DISCUSSION

- The model was implemented on the WEST<sup>®</sup> modelling and simulation software [3] (see Figure 3). Using the monitoring data of February and May 1998 [4], the model was calibrated [5] and validated (see Figure 4).

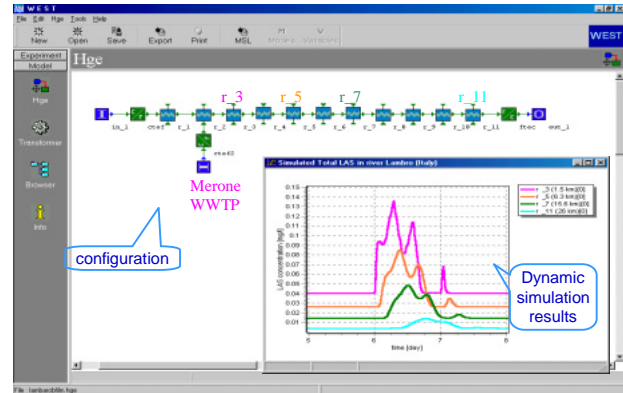


Figure 3. Chemical fate model in WEST<sup>®</sup> interface

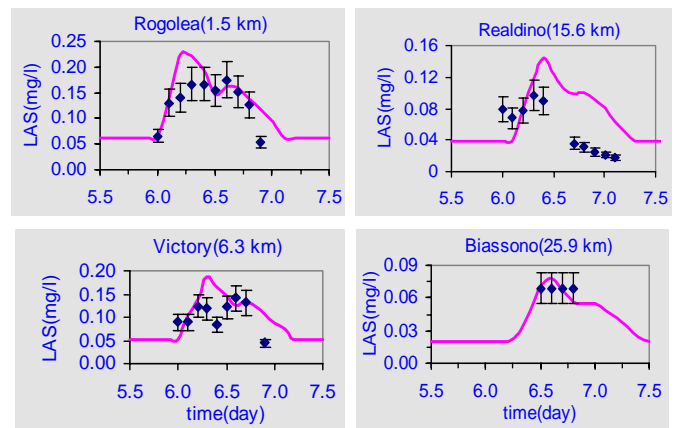


Figure 4. Model validation: measured (♦) and simulated (—) data sets in four river sections

- In both calibration [5] and validation (Figure 4) results, the general trend of simulated data sets agrees well with the measured data within 20% error.
- More reliable data can improve the model performance.
- As heterotrophic biomass density in the benthic sediment is higher than in the bulk water, biofilm biodegradation in the benthic sediment dominates the biodegradation process.

## TAKE HOME MESSAGE

- Dynamic exposure modelling is a realistic and feasible approach for time variable emissions.
- The model is relatively simple and detailed enough for short term simulation.
- The model can also simulate the concentration of sorbed LAS in the sediment.

## ACKNOWLEDGEMENT

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