

## REFINING AN IN-STREAM FATE MODEL OF ORGANIC CONTAMINANTS: A CASE STUDY OF LAS IN THE RIVER LAMBRO

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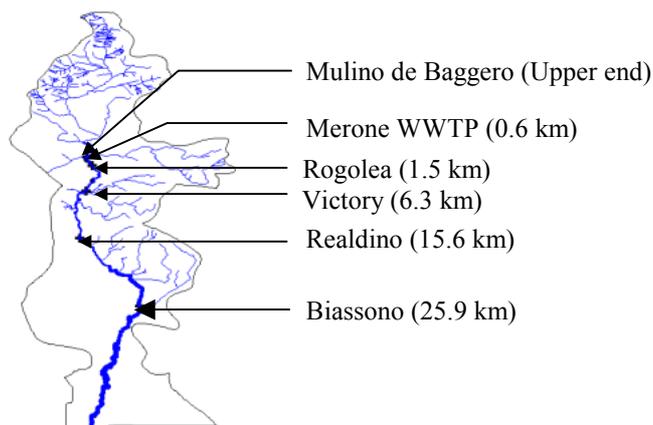
### INTRODUCTION

Most of the models describing the fate and transport of xenobiotic organic chemicals in natural streams are steady state models (e.g. *EXAMS*, *SYMPTOX4*, *GREAT-ER*,...). In view of ecological risk assessment, the current Predicted Environmental Concentration (PEC) estimation method in the European Union (EU) member states is based on a steady state in-stream fate model (OECD, 1999). These models assume continuous and uniform flow emissions, which is not justifiable as, in reality, the flow varies significantly with time. In such cases, a dynamic modelling approach is more realistic because it accounts for the temporal variability (Verdonck et al., 2002). Thus, the refinement of in-stream fate models is required for realistic exposure assessment.

Thus, the aim of this study is to develop a simple dynamic in-stream fate model using a multi-compartment approach. The model was evaluated on the basis of a LAS case study in the river Lambro, and the comparison of predicted and measured data sets is presented.

### STUDY SITE

The study was conducted at the river Lambro (in Italy). The site under consideration



**Figure 1.** Lambro River catchment with water quality measurement stations.

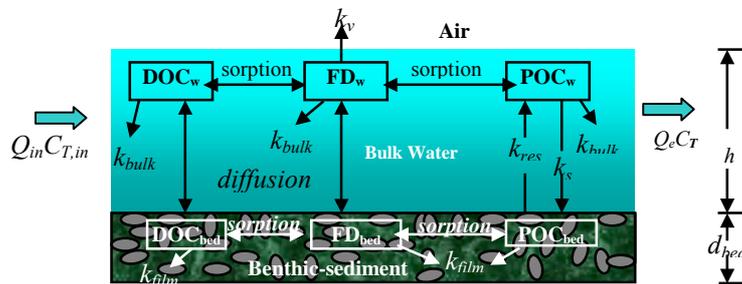
is limited to the part of the river Lambro between Mulino de Baggero (as upstream end) and Biassono (as downstream end) (see Figure 1). Downstream Mulino de Baggero, the most relevant pollutant discharge is from the wastewater treatment plant (WWTP) in Merone. The river receives variable WWTP effluent discharges and combined sewer overflows (CSOs) with a pollution equivalent of 118,200 inhabitants.

**MODEL FORMULATION**

In the model formulation, the complex hydrodynamic model was simplified to a series of completely mixed tanks in series (Beck and Reda, 1994). For the river Lambro case study, each river stretch was subdivided into a number of tanks in series (in total 47 tanks in series). For the water quality model, a simplified version of the River Water Quality Model number 1 (RWQM1) (Reichert et al., 2001; Dek-sissa et al., 2002) was applied and extended to include the fate of toxic organic compounds. As toxic organic chemicals behave differently in different environmental compartments, the river ecosystem was divided into three compartments: air, bulk water and benthic-sediments (see Figure 2). In the bulk water compartment, the chemical may be sorbed to Dissolved Organic Carbon ( $DOC_w$ ), suspended Particulate Organic Carbon ( $POC_w$ ), and freely dissolved in the bulk water ( $FD_w$ ). In the benthic-sediment, the chemical may be sorbed to DOC in the pore water ( $DOC_{bed}$ ) and Particulate Organic Carbon in the sediment ( $POC_{bed}$ ), or remain freely dissolved in the pore water ( $FD_{bed}$ ).

Mathematically, using an instantaneous local equilibrium assumption and first order kinetics, the general mass balance for concentrations of total LAS in the bulk water ( $C_T$ ) in every river tank, can be expressed as follows:

$$\frac{d(V C_T)}{dt} = Q_{in} C_{T,in} - Q_e C_T - (k_{bio\ deg} + k_V) f_d C_T V - k_{bio\ deg} f_{doc} C_T V - (k_s + k_{bulk}) f_P C_T V + k_{res} f_{P,bed} C_{T,bed} V_{bed} + K_L \left( \frac{C_{T,bed}}{\alpha_{bed}} - (1 - f_P) \cdot C_T \right) A$$

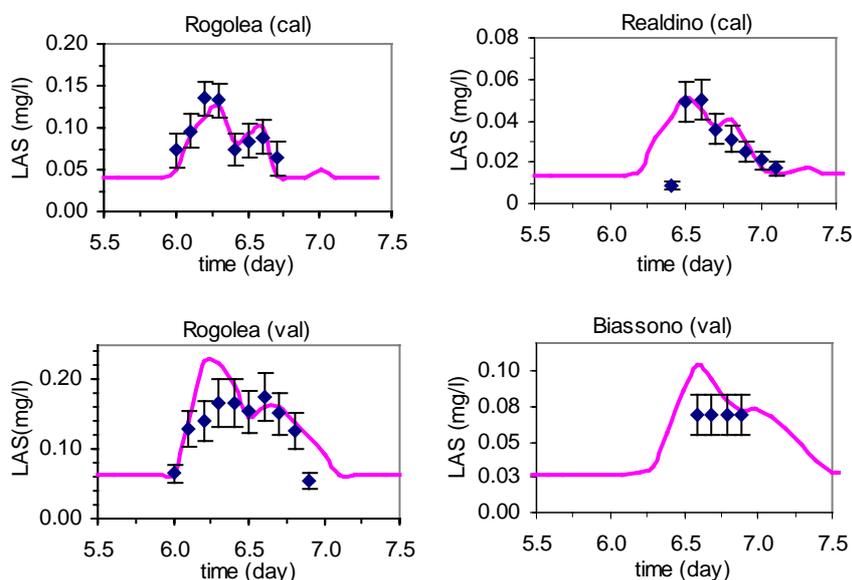


**Figure 2.** Schematic representation of the LAS in-stream fate model:  $h$  and  $d_{bed}$  are the depth of bulk water and active sediment layer (benthic-sediment), respectively.

where  $\alpha_{bed} = 1 + K_{P,bed} \cdot POC_{bed} + K_{doc,bed} \cdot DOC_{bed}$ ;  $V$  and  $V_{bed}$  are the volume of the tanks for the bulk water and the benthic sediment, respectively [ $m^3$ ];  $Q_{in}$  and  $Q_e$  are the inflow rate and the outflow rate, respectively [ $m^3 d^{-1}$ ];  $C_T$  and  $C_{T,bed}$  are the unfiltered/total chemical concentrations in the bulk water and in the benthic-sediment, respectively [ $g m^{-3}$ ];  $k_s$ ,  $k_v$ ,  $k_{res}$ , and  $k_{biodeg}$  are pseudo first order rate constants for respectively sedimentation, volatilization, resuspension, and overall biodegradation (in the bulk water  $k_{bulk}$  plus in the benthic sediment  $k_{film}$ ) [ $d^{-1}$ ];  $f_d$ ,  $f_p$  and  $f_{doc}$  are the fractions of respectively free dissolved LAS, and LAS sorbed to POC and DOC [-]; the subscript *bed* is indicating the benthic sediment, whereas *w* is for the bulk water;  $K_L$  is the mass transfer coefficient between the bulk water and the pore water [ $m d^{-1}$ ];  $K_{P,bed}$  and  $K_{doc,bed}$  are the partition coefficients in the river bed for sediment-water and DOC-water, respectively [ $m^3 g^{-1}$ ];  $A$  is the surface area of the river bed [ $m^2$ ];  $k_{film}$  is the pseudo first order biodegradation rate constant in the benthic sediment or biofilm [ $d^{-1}$ ].

## RESULTS AND DISCUSSION

The dynamic model was calibrated and validated on the basis of monitoring data taken in February and May 1998 (Whelan et al., 1999), respectively. Using the WEST<sup>®</sup> modelling and simulation software (Vanhooren et al., 2002), the results are illustrated in Figure 3. The LAS concentration predictions at different locations in the river Lambro generally agree well with the measured data sets within 20% error.



**Figure 3.** Model calibration (cal) and validation (val) results: simulated (—) and measured (◆) total LAS concentration in the bulk water.

The model also simulates the concentrations of sorbed LAS in the benthic sediment and in the pore water. The predicted sorbed LAS concentration in the benthic sediment is very low. Even though there is no information available about the LAS concentration in the benthic sediment of the river Lambro, the literature shows that the concentrations of LAS in the benthic sediment are generally very low (Feijtel et al., 1999).

## CONCLUSIONS

Based on the results obtained one can draw the following conclusions. As it takes into account the temporal variation, the proposed dynamic in-stream fate modelling is a realistic approach, and reduces the uncertainty of model results based on steady state assumptions. The fate and transport of toxic chemicals in different environmental compartments are different; the division of the river system into multi-compartments is justifiable. The model is relatively simple and detailed enough to express the short-term (daily) temporal variation of LAS in the river environment. As the instantaneous local equilibrium assumption is limited to contaminants with a rapid desorption equilibrium, care must be taken while applying this model for short-term simulation (e.g. hourly).

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