COMPARISON OF NUMERICAL TECHNIQUES SOLVING LONGITUDINAL DISPERSION PROBLEMS IN THE RIVER MONDEGO

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ABSTRACT

Judicious selection of mathematical models for application in a specific river basin management can mitigate prediction uncertainty. Therefore, intervention times will be established with better reliability and alarm systems could efficiently protect the aquatic ecosystems and the public health. The main purpose of this paper is to evaluate the performance of different numerical techniques when applied to river water systems dispersion modelling. A case study was developed to assess the environmental impact of Urgeiriça mining waters in a Mondego river reach, between Caldas da Felgueira and Aguieira reservoir. A monitoring program was carried out using tracer injection (rhodamine WT) to determine the *in situ* dispersion river water behaviour. The present work describes the methodology used in the tracer experiments, presents the concentration-time curves obtained and the performance of finite difference method (FDM) and finite element method (FEM) in a simplified river system, and compares the results of different numerical techniques application for longitudinal dispersion coefficient estimation in this river reach. The application of DUFLOW package, that includes hydrodynamics and water quality models, showed the best agreement with experimental data, allowing a reasonable support for impact assessment of different discharges scenarios in the river water quality.

KEYWORDS

Environmental impact assessment, longitudinal dispersion, mathematical models, numerical methods, rhodamine WT, river Mondego, tracer experiments, water quality, water resources management.

INTRODUCTION

River hydrodynamics and pollutants discharges dispersion are determinant factors in river basin planning and management, when different waters uses and aquatic ecosystems protection must be considered. The ever increasing computational capacities provides the development of powerful and user-friendly mathematical models for simulation and forecast receiving waters quality changes after wastewater discharges and land runoff.

The aims of this paper are to evaluate the performance of different numerical techniques when applied to pollutant transport modelling in a Mondego river reach (Figure 1), and to estimate longitudinal dispersion coefficients in river water. Run-off from Urgeiriça uranium mine discharged to Pantanha streamlet, a tributary of river Mondego, has determined the interest of an environmental impact assessment on receiving waters.

A monitoring program was carried out using tracer injection (rhodamine WT) to evaluate the *in situ* dispersion river water behaviour under three different flow regimes: flood (100-144 m^3s^{-1}), dry-weather (0,65-0,75 m^3s^{-1}) and frequent (28-40 m^3s^{-1}) conditions. For operational convenience, dye tracer was discharged in two different river sections and the water samples were collected at several sites downstream. With observed concentration data (under frequent flow regime), three models were calibrated in order to produce operational tools to define how long water abstractions need to be suspended after a spill, the probabilistic arrival/peak/recession times, and pollutant concentrations.

The performance of two models (DUFLOW and ConvDiffFEM) using different numerical methods (FDM and FEM, respectively) applied to a simplified system were compared in order to assess their relative accuracy. Indeed, the differences of the obtained results shown that FDM solving longitudinal dispersion problems is accurate enough when compared with the more sophisticated numerical based on FEM. Therefore, two finite difference models (DUFLOW and ADZTOOL) using different numerical techniques were applied for longitudinal dispersion coefficients estimation. The comparison of the agreement between experimental data and obtained model results allows the conclusion that DUFLOW is the most accurate used model. A validation of this model was carried out, for flood flow regime observed concentrations, in order to evaluate its accuracy describing and predicting conservative pollutant transport under different hydrodynamic conditions.

STUDY AREA

The Mondego river basin is located in the central region of Portugal, confronting with Vouga, Lis and Tagus, and Douro river basins, from north, south and east, respectively. The drainage area is 6670 km^2 and the annual mean rainfall is between 1000 and 1200 mm.

The study area occupies the medium part of the basin and is distributed over six municipalities: Nelas, Carregal do Sal, Santa Comba Dão (right side), Seia, Oliveira do Hospital e Tábua (left side). The river reach considered in this study begins downstream Caldas da Felgueira bridge and ends at Tábua bridge, in a distance of approximately 24 km. Main tributaries are river Seia and river Mel. The water is intensively used for hydropower generation, domestic and industrial water supply and agricultural irrigation.

The average reach bottom slope is 0,9 ‰. Seven sampling sites were considered, being the site 0 (Caldas da Felgueira bridge) the upstream dye tracer injection point, where is located the unique gauge station in this reach and before Aguieira dam. Water levels at Aguieira reservoir were recorded during the monitoring program.

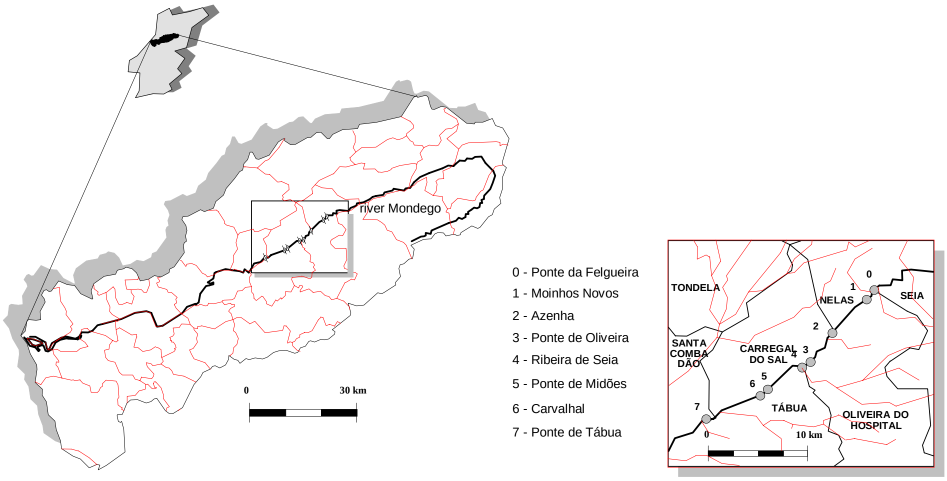

Figure 1: General layout of Mondego river basin and sampling sites localisation

METHODOLOGY

The dye tracer used in this study was rhodamine WT (20% solution), recommended by its characteristics: not toxic, not reactive, good diffusivity, high detectability, low sorptive and acidity. For concentrations measurements a "Turner Designs" fluorometre was used. Blanks are taken in all sampling sites for river natural fluorescence determination.

Sampling sites location (Figure 1) were established according to the aims of this monitoring program, the sites accessibility (bridges), river physics characteristics, mixing conditions, weirs location, logistical means and human resources availability. Table 1 presents the information about all the tracer injections on the three sampling programs made in this study.

TABLE 1

SYNTHESIS OF TRACER INJECTIONS INFORMATION

Injection	Date	Hour	Point	Flow (m^3/s)	Rhodamine mass (g)
1	89-12-09	8:20	Site 0	140	100
2	89-12-09	15:40	Site 3	144	200
3	89-12-10	8:00	Site 0	100	200
4	89-12-10	8:30	Site 5	110	400
1	90-06-15	7:32	Site 0	0.74	400
2	90-06-15	8:30	Site 3	0.74	200
1	90-11-09	7:40	Site 0	40	400
2	89-11-10	8:00	Site 3	29	400

Experimental longitudinal dispersion coefficients were calculated from concentration-time curves at consecutive sampling sites, using the methodology described by Chapra (1997) for tracer studies. With this values, an analytical solution of advection-diffusion equation (Eqn.1), where the conservative substance is initially concentrated at x=0 was performed and compared with the numerical solution.

$$\frac{\partial C}{\partial t} = -U\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} \tag{1}$$

where,

t	Time	[T]
C	constituent concentration	$[ML^{-}]$
x	distance as measured along the channel axis	[L]
U	mean velocity (averaged over the cross-sectional area)	$[L^{1}T^{-1}]$
D	Longitudinal dispersion coefficient	$[L^{2}T^{-1}]$

The dye tracer injected mass recovered at each sites allows to assess the importance of physical and biochemical processes by quantification of precipitation, sorption, retention and assimilation losses.

The discharges values considered for calculations are obtained from Nelas flow gauge station records. Mean water velocity in reaches were calculated with mean travel time and distances between sampling sites (Table 2).

TABLE 2
DISTANCE BETWEEN INJECTION POINTS AND SAMPLING SITES

SAMPLING SITES	Distance from injection points		
	Site 0	Site 3	Site 5
1	1.250	—	—
2	6.200	—	—
3	11.000	—	—
4	11.650	650	—
5	16.700	5.700	—
6	17.400	6.400	700
7	24.000	13.000	7.300

The flow regime of this river reach is strongly influenced by the Aguieira reservoir water level and by the fourteen weirs considered, as shown in Figure 2.

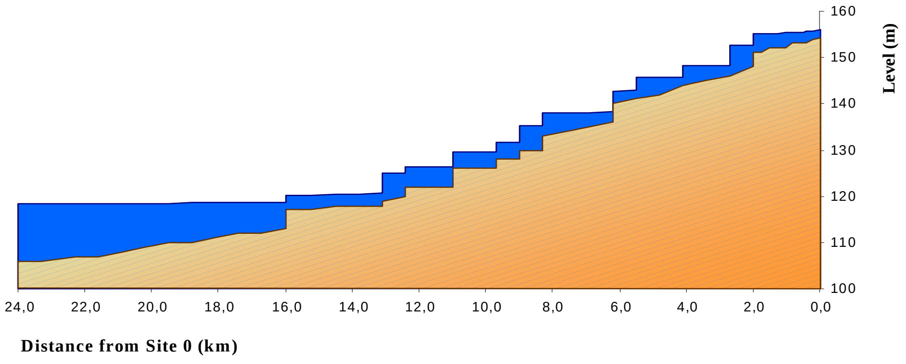

Figure 2: River longitudinal profile

MODELS

DUFLOW model

DUFLOW model was designed to cover a large range of applications in different water systems and to assess water quality problems (ICIM, 1992).

The package is based on the one-dimensional partial differential equation that describes non stationary flow in open channels. These equations, which are the mathematical translation of the laws of conservation of mass (Eqn.2) and of momentum (Eqn.3).

$$A\frac{\partial H}{\partial t}+\frac{\partial Q}{\partial x}=0 \tag{2}$$

$$\frac{\partial Q}{\partial t}+gA\frac{\partial H}{\partial x}+\frac{\partial(\alpha QU)}{\partial x}+\frac{g|Q|Q}{K_C{}^2 AR}=0 \tag{3}$$

where:

H(x,t)	water level with respect to reference level	[L]
Q(x,t)	discharge at location x and at time t	$[L^3T^{-1}]$
R(x,H)	hydraulic radius of cross-section	[L]
A(x,H)	cross-sectional flow area	$[L^2]$
b(x,H)	cross-sectional flow width	[L]
G	acceleration due to gravity	$[L^1T^{-2}]$
K_C (x,H)	coefficient of De Chezy	
α	correction factor for non-uniformity of the velocity distribution	

The Eqn.(2) states that if the water level changes at some location this will be the net result of local inflow minus outflow. The Eqn.(3) expresses that the net change of momentum is the result of interior and exterior forces like friction and gravity, when the wind action is neglected.

The water quality part of the DUFLOW package is based on more general form of the Eqn.1 presented in the Eqn.4. This partial differential equation describes the concentration of a constituent in a one dimensional system as function of time and place. The “production” term (P) includes all physical, chemical and biological processes to which a specific constituent is subject to. The process descriptions can be supplied by the user, that can create different types of kinetics.

$$\frac{\partial(AC)}{\partial t}=-\frac{\partial(QC)}{\partial x}+\frac{\partial}{\partial x}(AD\frac{\partial C}{\partial x})+P \tag{4}$$

The Eqn.(2), (3) and (4) are discretized in space and time using the four-point implicit Preissmann scheme. This scheme is unconditionally stable, shows little numerical dispersion, and allows non-equidistant grids. It computes discharges and elevations at the same point. Furthermore the method perfectly fits to the discretization of the flow equations.

DIFFPACK module (ConvDiffFEM)

This module is a simulator, built on the DIFFPACK system, for scalar convection-diffusion problems, based on object-oriented programming.

The main application of this code is probably rapid establishment of a finite element solution in a given convection-diffusion problem. The simulation model is defined in terms of the governing partial differential equations and the associated initial and boundary conditions. For one-dimensional problems, the equation to be solved is similar to Eqn. (4), considering constant the discharge flow and the cross-sectional flow area.

The boundary conditions are of three types: essential conditions (*C* is prescribed); natural Neumann conditions; and natural Robin condition. The initial condition $C(x_1, \dots, x_d, 0)$ is given as a function of the spatial coordinates. The initial-boundary value problem is solved by a finite element method where the weighting functions are allowed to be different from the trial functions. The approximation can be given by (Langtanden, 1995)

$$C \approx \overline{C} \equiv \sum_{i=1}^{n} N_i(x_1, \dots, x_d) C_i(t) \tag{5}$$

where,

N_i	prescribed finite element trial functions
$C_i(t)$	functions (concentrations) to be found by the method

For spatial discretization a weak formulation of the mathematical problem is used. Temporal discretization is carried out by the so called “theta-scheme”. For the equation $d\psi/dt=g$, the time derivative, for time level *r*, is approximated according to,

$$\frac{\psi^r - \psi^{r-1}}{\Delta t} = \theta g^r + (1-\theta) g^{r-1} \tag{6}$$

AGGREGATED DEAD ZONES (ADZ) model

The ADZ modelling technique is a relatively recent approach to modelling dispersion processes that provides accurate predictions of the time travel and spread moving downstream in a natural stream (Lees and Camacho, 1998). For advection/dispersion parameters estimation, a simple method (ADZTOOL) uses derived relationships from observed concentration-time data measured at two downstream locations (Wallis et al.,1989), for simulate the effects of conservative solute transport in a river reach.

This simple deterministic methodology does not involve any optimisation. The first order discrete-time model implemented is only an approximation of the governing differential equations. Parameters estimation only derived from experimental data (with some errors), because there is no hydrodynamic module coupled with ADZTOOL. For each observed distribution, the time of first arrival (τ_i), centroid location (t_i), the mean travel time ($\bar{t}$), the time delay (τ) and ADZ residence time (T) are calculated for each reach between consecutive sampling stations. After parameters calculation, the response of a first order discrete ADZ model is computed by the equation,

$$C_k = -a\, C_{k-1} + b_0\, C_{0,\, k-\delta} \qquad (7)$$

where,

C_k	output concentration at sampling interval (k)
C_{k-1}	output concentration at the previous sampling interval
$C_{0,\, k-\delta}$	input concentration at the sampling interval (k-δ)
δ	advective time delay in sampling intervals
a , b_0	coefficients of the first order discrete transfer function, given by $a = -\exp(-\Delta t/T)$ and $b_0 = 1+a$.

RESULTS AND CONCLUSIONS

Experimental results

Tracer concentration of samples collected after the first injection of November 90 monitoring program are depicted in Figure 4.

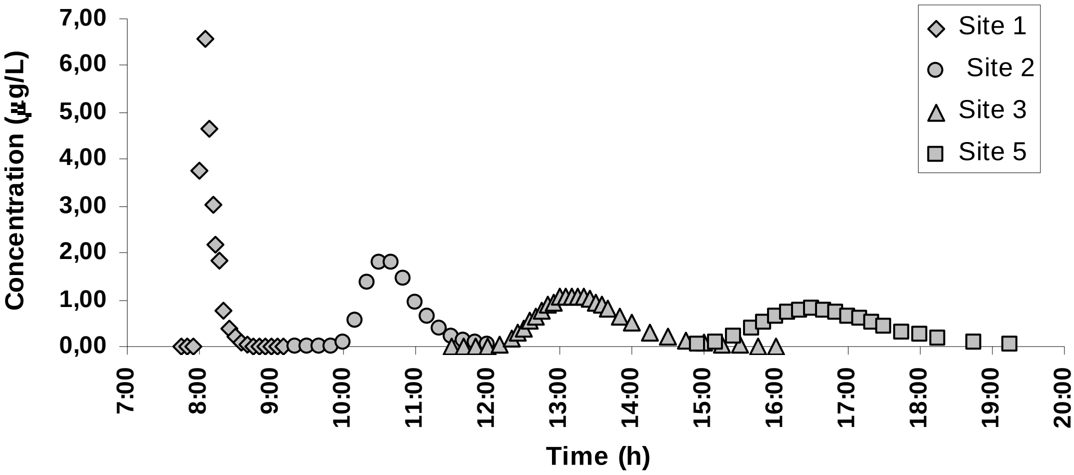

Figure 4: Experimental results of November-90 monitoring program (1st. Injecction)

Comparison of different numerical methods (FDM and FEM)

DUFLOW model (based on FDM) and ConvDiffFEM model (based on FEM) were applied to a simplified open channel (with the same length of the monitored river reach and constant geometric properties) in order to assess FDM and FEM performance. Flow was considered constant in time and space. Output of this simulation procedure is presented in Figure 5, where the correlation coefficients values denotes a good agreement between the two model results.

Furthermore, DUFLOW model requires less computation time then ConvDiffFEM model, and solves simultaneously the hydrodynamic equations, which is a determinant property to deal with longitudinal transport and dispersion problems.

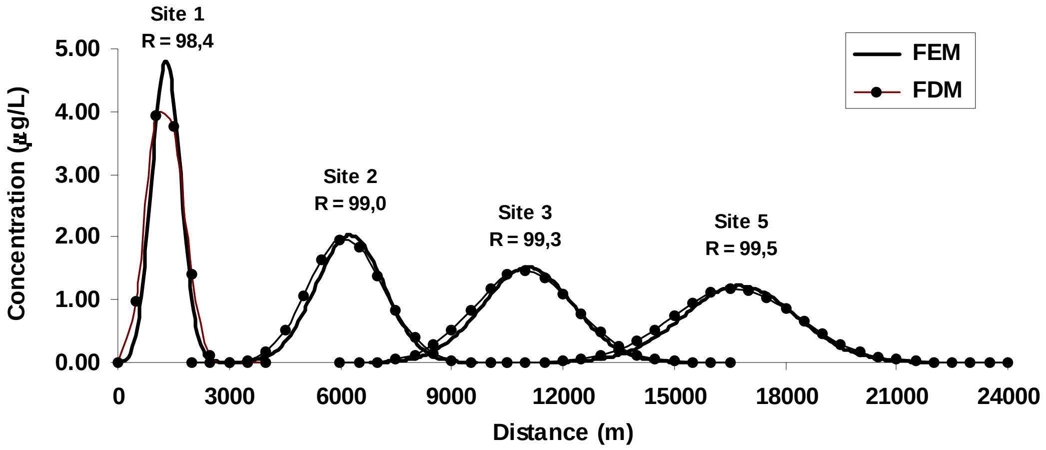

Figure 5: Agreement between DUFLOW and ConvDiffFEM model results

Comparison of different FDM numerical techniques

The previous described FDM models (DUFLOW and ADZ) were applied to the studied river reach in order to assess numerical techniques performance reproducing the observed river dispersion behaviour. Figure 6 shows the agreement between experimental concentration-time curves with model outputs and analytical solution results, at the four sampling sites considered in the first injection of November-90 monitoring program.

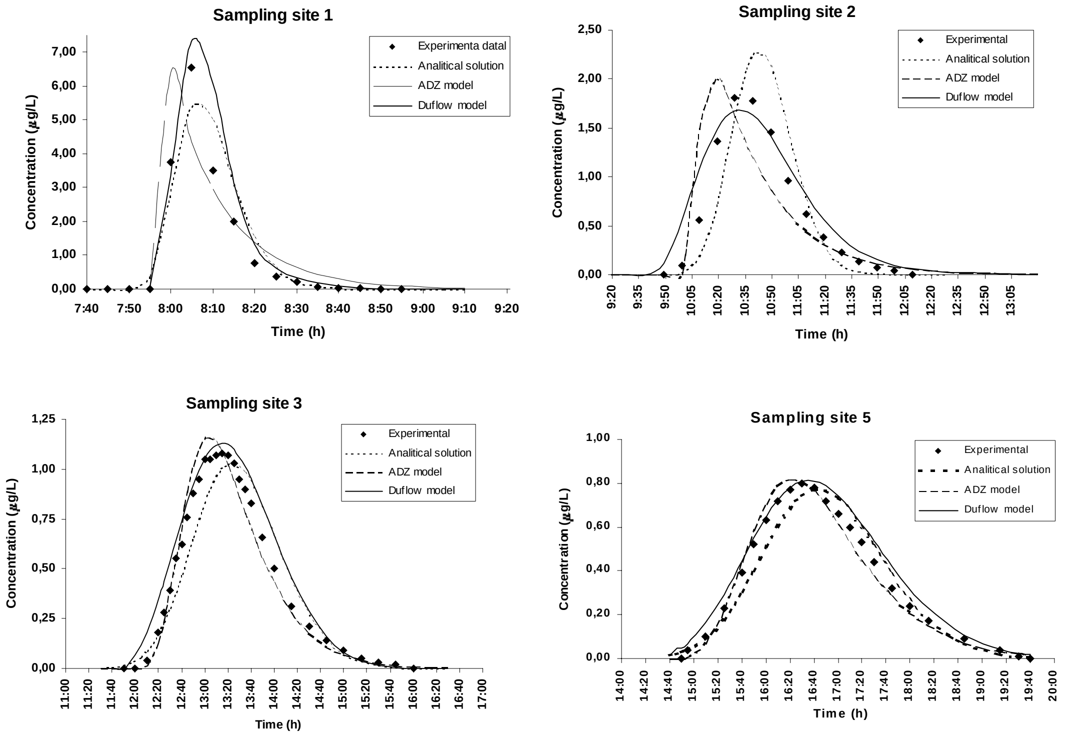

Figure 6 – Comparison of models results and experimental data

A good agreement of both numerical models with experimental data and a relatively better performance of DUFLOW model can be inferred from these graphics. This conclusion can be supported with the correlation coefficients values calculated for the three used models (Figure 7).

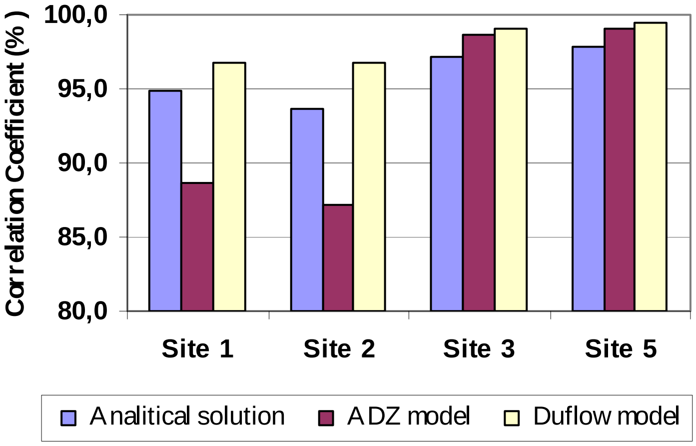

Figure 7: Models results agreement with experimental data

Table 3 compares mean velocity, travel time and dispersion results obtained from DUFLOW and ADZ models with tracer experimental data. It is apparent little differences between the longitudinal dispersion coefficients calculated from experimental data (Thomann and Mueller, 1987) and the values adopted for DUFLOW model calibration. A sensitivity analysis has shown that these differences do not affect significantly the simulated concentration and travel time values.

TABLE 3
COMPARISION OF NUMERICAL MODELS RESULTS

REACH	MEAN VELOCITY (ms^{-1})			TRAVEL TIME (s)			DISPERSION COEFFICIENT (m^{2}s^{-1})		
	EXPE.	ADZ	DUFLOW	EXPE.	ADZ	DUFLOW	EXPE.	ADZ	DUFLOW
E1 – E2	0.526	0.548	Var.	9407	9035	9290	14	43	10
E2 – E3	0.497	0.502	Var.	9660	95554	9634	51	25	45
E3 – E5	0.473	0.473	Var.	12043	12504	11912	37	36	35
E1 – E3	0.511	0.524	Var.	19067	18589	18924	34	33	-
E1 – E5	0.497	0.504	Var.	31110	30643	30836	35	35	-

DUFLOW model validation

DUFLOW model has been validated using experimental data from December-89 monitoring program first injection, under flood flow conditions. A good agreement is also obtained (Figure 8).

For this flow regime longitudinal dispersion coefficients values range from 60 to 110 m^{2}s^{-1}.

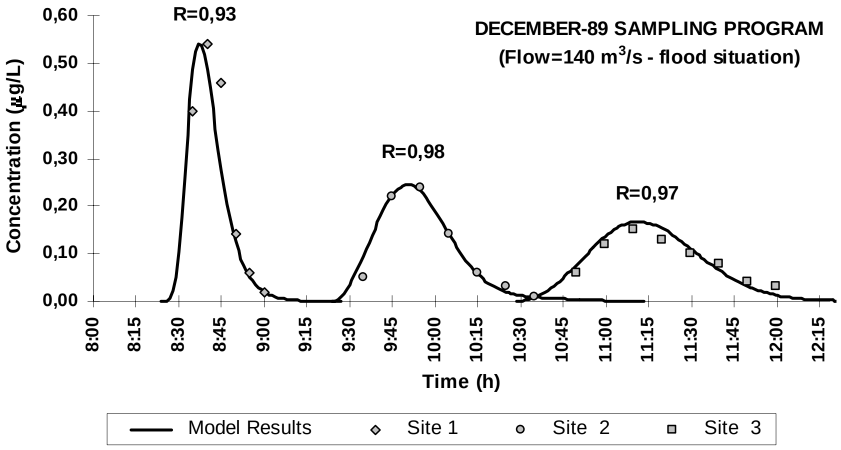

Figure 8: Duflow model validation

One-dimensional mathematical modelling revealed to be a powerful and accurate tool to solve pollutant transport problems in river systems with a dispersion behaviour similar to the studied river reach, even under different flow regimes

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