Experiences in water quality simulations of a mediumsized agricultural temporary river basin

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1 Introduction

Analysis of the behaviour of temporary rivers is a complex multi-dimensional task, but the help of modern modeling software may be a promising aid in this effort. Different temporal scales have to be considered, ranging from long term accumulation periods in the order of months or years to the finer scale during the onset of the transporting (flow) period whose most important period may not last more than hours or days. Spatial issues play a role especially in fluxes for particulates: hot spots, built during the dry period can be successively transported downstream altering the concentration severely while passing through a measuring gauge, so there is a high degree of uncertainty.

Instream concentration of pollutants depends on the complex interaction of dissolved and particulate nutrients and their consumers. During the dry period, turnover rates, mostly directly bound to concentration values, are very sensitive to even minor inflows which disturb the settled, equilibrium system. A lot of models have been already developed for more humid environments, and simulations were already applied for the Thau lagoon in France to evaluate long term nutrient balances (Chapelle, 1995; La Jeunesse et al., 2002), also taking into account the simulations of the delivering rivers (Plus et al., 2006).

In order to continue this effort a new model was developed during the European project tempQsim. This tempQsim – STREAM model was based on the framework of the MOHID Water Modeling System, described e.g. in (Miranda et al., 2000) or (Trancoso et al., 2005). Then it was applied to the Véne river to model the instream accumulation processes in a medium time scale with a special focus on first flush loadings of volatile suspended solids (VSS) caused by thick organic layers of bacteria and algae downstream treated waste water inflows during the dry phase.

2 Methods

2.1 MOHID Water Modelling System and the tempQsim STREAM model

2.1.1 General

The development of MOHID started in 1985 and was initially a two-dimensional tidal model written in FORTRAN 77 (Neves, 1985). At this time it was focused on studying estuaries and coastal areas using a classical finite-differences approach. In the following years, two-dimensional eulerian and lagrangian transport modules were included in this model and the concept of a finite volumes approach was introduced to replace the FDM. It is currently maintained and developed by the MARETEC (Marine and Environmental Technology Research Center) group of the Instituto Superior Técnico (IST) at the Technical University of Lisbon. Up to now, it was constantly enhanced by additional features and modules.

2.1.2 Framework of the model

There are three core tools: (i) MOHID Water, (ii) MOHID Land and (iii) MOHID Soil.

The first tool is the improved version of the original tidal model, the second one is a watershed model and the third one simulates water flow through porous media.

All models share the same framework of post- and pre-processors and can therefore easily be coupled or substituted by others. During the European project tempQsim (Contract no: EVK1-CT2002-00112), the river network part of MOHID Land was developed and enhanced further under the synonym *tempQsim STREAM model*.

The tempQsim STREAM model consists of a hydrodynamic model which can be coupled with a non-steady state water quality model and a benthic model.

The model was reorganized in 1998, using an object oriented conceptualisation in ANSI FORTRAN 95 as described in (Decyk et al., 1997) and (Miranda et al., 2000).

2.1.3 Flow routing

The hydrodynamics can be computed with the kinematic wave, diffusion wave or the full Saint-Venant equations. The solution can be done implicit (with the approach similar to CASCADE) or explicit. In this study, only the explicit kinematic wave approach was applied.

Downstream boundary can be null gradient, a dam, or an imposed level at the outlet node.

The timestep can be either set to a constant value or defined in terms of a maximum and minimum value, so that numerical stability is always sustained.

2.1.4 Water quality

The water quality module is a zero-dimensional ecological model which was developed based on WASP (Wool et al., 1993) and further enhanced. It now considers 18 parameters as shown in Table 1.

Table 1: Considered state variables in the tempQsim model

0	particulate organic nitrogen	0	dissolved oxygen
0	dissolved refractory and non	0	biochemical oxygen demand (BOD)
	refractory organic nitrogen	0	temperature
0	ammonia, nitrate, nitrite	0	salinity
0	particulate organic phosphorus	0	cohesive sediment (3 fractions)
0	dissolved refractory and non		
	refractory organic phosphorus	_	Tee J Vee
0	inorganic phosphorus	0	155 and V55
0	phytoplankton	0	algae
0	micro- and macrozoobenthos	0	heterotrophic bacteria

Water properties are described by an advection diffusion equation including a settling and erosion term in case of particulate suspended matter. Diffusion is quantified by Fick's Diffusion Law.

2.1.5 Particulate transport and benthic processes

A benthos module has been developed to compute biogeochemical processes in the benthic zone at the water-sediment interface. Particulate phases can settle and deposit at the river bed and will there be subject to further conversion. Several processes can be computed, including:

- o algal mortality
- particulate organic matter mineralization

- o biogenic silica dissolution
- o oxygen depletion
- growth of heterotrophic bacteria in the river bed (often caused by point source inputs in dry phases where shear stresses are low).

The erosion algorithm is based on the approach of (Partheniades, 1962), deposition on the algorithm which was first proposed by (Krone, 1962) and later on modified by (Odd and Owen, 1972).

The approach was further modified to account for hiding ability of fractioned sediment.

2.2 Extension of the tempQsim model

2.2.1 Bacterial growth in pools

During the dry phases, the Vène has greatly increased growth of bacteria downstream of the point source inflows. Due to constant inputs through the WWTPs into the pools and the very low stream velocity, an accumulation of organic matter takes place on the river bed and in the riparian zone. This accumulated matter seems to be responsible for increased loadings during the onset of early autumn floods.

In order to account for this accumulation, the tempQsim model was extended. Bacterial concentration has been defined as a particulate property and is therefore enabled to sink to the bottom. On the river bed (represented by the module benthos in the model) the bacteria can continue growth by consuming particulate organic matter (POM) and dissolved non-refractory organic matter (DONnr) as shown in Figure 1. Dead bacteria are then converted into refractory particulate organic matter (POMr).



Figure 1: Scheme for processes of heterotrophic bacteria introduced in MOHID

2.2.2 Fractioned sediment transport

Temporary rivers are characterized by highly varying stream velocities. Dry phases with hardly any movement alternate with flash flood events. In the original version of the model, cohesive mineral sediment was only considered as one fraction. In order to account for the great variability in velocity (which is one main driver of sediment transport capacity), the module was extended to include two additional sediment fractions. For each of the three fractions, parameters such as fall velocity, critical shear stresses for erosion and deposition, erodibility etc. can be chosen or will be computed independently.

2.2.3 Calculation of TSS and VSS

In order to simplify calibration and comparison with commonly measured parameters, the properties total suspended solids (TSS) and volatile suspended solids (VSS) were added (EQ. 2-1 and EQ. 2-2).

$$TSS = \sum_{i} cohesive \ sed_{i} + VSS$$
EQ. 2-2

VSS is the sum of all transported particulate organic living and dead matter and TSS is the sum of VSS and the mineral sediment fractions.

2.2.4 New calculation of available erosion capacity for each fraction

Although only a single mineral sediment fraction was included in the original version of the tempQsim model, it already allowed the calculation of more than one particulate state variable as there were a couple of particulate organic properties. To account for differences in the availability on of bed material, the erosion rate was formerly normalized by the mass (resp. bottom concentration in ML⁻²) of cohesive sediment. The error introduced by this was considered to be negligible, because the concentration of cohesive sediment was assumed to be magnitudes higher than the concentration of particulate organic materials.

In the case of temporary waters, their capacity for mass retention and biomass accumulation, this assumption may no longer be valid. The introduction of TSS now allows a better distribution of the available transport capacity for each constituent depending on the proportion of mass of the totally available particulate matter (TSS). The erosion rate according to (Partheniades, 1962) has therefore been modified as follows

$$\boldsymbol{E}[\boldsymbol{i}] = \boldsymbol{M}_{e}[\boldsymbol{i}] \left(\frac{\tau_{b}}{\tau_{crit,e}[\boldsymbol{i}]} - 1 \right) \cdot \left(\frac{property[\boldsymbol{i}]_{bottomconc}}{TSS_{bottomconc}} \right)$$
EQ. 2-3

where

Due to their reference to the mass density on the bottom, the formula in EQ. 2-3 accounts indirectly for the amount of erosion activity which is dissipated by the regarded fraction, but disregards the spatial availability.

3 Application and Results

3.1 Spatial discretisation

The model was applied to the Vène catchment which has already been presented, e.g. in (Tournoud et al., 2006; Tournoud et al., 2005). In the modelling, only the main branch of the river between points K (karstic spring Cournonsec) and V are considered.

Based on the spatial discretisation of the DEM (Digital Elevation Model) consisting of a regular orthogonal grid with a side length of 50 m, a river network was delineated. The network has 360 reaches with element lengths from 50 to $50x\sqrt{2}$ m and trapezoidal cross sections of 3 to 6 m width.



Figure 2: Spatial discretization of the Vène in MOHID-GIS

The model of the river has 5 main point source inflows: the karstic spring Cournonsec (K) at the top of the river, a winery (b), an agricultural area (c) as well as the two wastewater treatment plants for Gigean and Montbazin (d and h). The delivery part of the model was calculated with the French model Mercedes or a simple storage cascade and is handed over to the simulation via defined inflow points at L, M, P, S, R, T and V. For the inputs of the WWTPs and the karstic spring at K, the water quality parameters are variable over time, if available by continuous measurements, if not (as e.g. for the overland flow), they were chosen constant.

3.2 Calibration issues

The system was calibrated on the basis of the hydrological year 2002/2003 and later validated on the year 2003/2004. Especially the first flush events on 2003-09-22 and 2004-09-13 were investigated. These floods have two different origins (one is dominated by the influence of the karst at K the other depends mainly on overland runoff which complicates the validation. For the simulation, a value of n=0.05 was chosen, as it is also often recommended for "natural rivers" with light brush.

Due to the absence of measurements for the hydraulic conductivity of the channel bed, the transmission losses had to be estimated. This was done on the basis of July 2004. In this month, the pool which was formed by the WWTP at Montbazin (d) (mean flow of about 0.006 m³/s) was approximated with a mean length of about 500m. The cross section in this part of the river has a steep, nearly rectangular trapezoidal shape with a width of 3 m. To balance the inputs of the WWTP, the transmission losses should equal the inflow of 0.006 m³/s for the regarded section, otherwise, the pool would overflow. On the basis of the assumption that seepage losses are the most important losses (normally one order of magnitude higher than evaporation), a hydraulic conductivity near $5x10^{-6}$ m³/(m²s) seemed to be appropriate.

The following scenarios were computed with the cascade retention as shown in Scholz (1995) and a storage constant of 50 min estimated after Euler (1978) and a runoff coefficient of 0.015.

3.3 Scenarios for the modeling

In order to define the overall performance of the model the following 11 scenarios have been calculated:

1)	all:	the parameterisation uses all processes explained in Chapter 2.1
2)	no transmission losses:	the main instream transmission loss, the infiltration, is turned off
3)	no bacteria:	inflow and growth of bacteria is turned off in the water phase as well as in the benthos
4)	no benthos:	the calculation in the benthos module is turned off, no processes occur at the river bed, but settling and resuspension are still possible
5)	no fraction:	instead of three sediment fractions, only one is calculated with a comparable parameter set and similar concentration in the inflows
6)	double WWTP:	concentrations of organic properties are doubled in the two WWTP effluents
7)	no WWTP:	concentrations of all properties of the WWTP effluent are set to zero (except temperature)
8)	no delivery:	concentrations of all properties of the delivery model are set to zero (except temperature), but the water inflow remains
9)	no karst:	concentrations of all properties of the karstic spring at K (Cournonsec) are set to zero (except temperature), but the water inflow remains as in 8)
10)	no processes:	all parameters are considered to be conservative, so they are only subject to advection, diffusion and settling or resuspension, but not to reactions in module water quality
11)	variable delivery WQ:	an approach was used to increase the runoff concentration with increasing dry days, i.e. the longer the dry period, the higher the concentrations; if a rainfall event occurred, concentrations were reduced up to a defined base level

Every scenario was executed on the same spatial discretisation for the hydrological years 2002/2003 and 2003/2004. The boundary conditions and parameter sets of the other scenarios are all based on scenario 1. The aims of the following model exercise is the definition of critical processes as well as their sensitivity and the agreement of the simulation with the measured values, with a focus on organic accumulation and resuspension expressed by volatile suspended solids (VSS).

3.4 Event scale simulation and results

Apart from the fluctuation on the annual timescale, there exists also an important inter-event dynamic.

3.4.1 Pollutographs for the event at 2003-09-22

Figure 3 and Figure 4 show the results of the first scenario ("all") in comparison to measured values for some of the output parameters at S on the first flush flood in September 2003.

The measured behaviour of the system could not always be represented in the simulation, especially concerning the delivery part. Calculations with the French model MERCEDES revealed a runoff coefficient of about 6 %, which was normally 1% for other floods (Perrin, 2006). Due to this, the first major peak in the flow, which is assumed to be caused by instant runoff at the start of the rain event could not be modelled.



Figure 3: Measured and simulated concentrations at Sanglier (S) for 2003-09-22, Scenario "all" for particulates and dissolved inorganic nitrogen

However, it must be noted that about 90-99% of the flow at S is contributed by the karstic spring at K during this event ([flow_S-transmissionloss_{K-S}]/flow_K). This means that it depends on the parameter, if this lack of compliance is serious for the overall mass transport or neglectable. For example, nitrate-nitrogen is mostly transported by the karstic spring with comparably high fluxes, whereas VSS or other organic compounds emerge other sources or are build up in the pools. So the effect on nitrate-nitrogen will be much smaller than on VSS in terms of the overall event load.



Figure 4: Measured and simulated concentrations at Sanglier (S) for 2003-09-22, Scenario "all" for inorganic phosphorus, particulate (organic) phosphorus and (particulate) organic nitrogen

Results at V were not included here. One main source, the Issanka spring at site K' could not be included in the model, because it is not possible to measure the volume of the contribution of this very diffuse spring. Even though the peak for VSS at S could be reproduced, there still seem to be additional sources of organic matter in the reach apart from the instream bacteria growth. This may be caused by the surrounding vegetation which is importing organic matter in the form of leaves and small branches and other detritus.

The courses of the other parameters seem in the range of normal applications. In the measurements, ammonia is slightly less concentrated in the beginning (Figure 3). Maybe the nitrification is more intensive than specified in the model. Particulate organic phosphorus along with particulate organic nitrogen is good approximated, only the peak is smaller in the simulation as it happened also with VSS (Figure 4).

3.4.2 Pollutographs for the event at 2004-09-13

As it was mentioned before, this flood is only caused by overland runoff. So limited replication of the delivery part will be even more obvious than before. Consequently, the water flux is strongly underestimated in the simulation of this flood as shown in Figure 5.



Figure 5: Measured and simulated concentrations at Sanglier (S) for 2004-09-13, Scenario "all" for particulates and dissolved inorganic nitrogen

This fact will have minor influence on the concentrations of solubles, as long as they are governed by the inflows, but it leads to an underestimation of the loadings charged to the receiving lagoon. If a particulate property as TSS or VSS is considered, the resuspension adds an additional error source, if flows are not calculated correctly. The concentrations of TSS are therefore underestimated, either due to a under representation in the inflows or by the missing transport capacity.

Ammonia underlies an early flushing followed by a fast dilution in the measurements, which is not reproduced by the model in this extend. The lacking dilution effect of rain on the overland runoff needs to be accounted for. Furthermore unclear remains the increase of the nitrate concentration in the falling limb of the hydrograph in the measurements. Either this is a cause of some delayed flows from instream nitrate storages in upstream pools or more likely by nitrate leaching from the soils.



Figure 6: Measured and simulated concentrations at Sanglier (S) for 2004-09-13, Scenario "all" for inorganic phosphorus, particulate (organic) phosphorus and (particulate) organic nitrogen

The course of POP and PON is better as it can be seen in Figure 6. There is a lot of fluctuation especially in the particulate phosphorus (PP) measurements, so the model's performance is in an acceptable range. As with ammonia, the dilution caused by the rainwater in the later stage of the flood was not accounted for (the delivery part is run with constant concentrations), so the concentrations are overestimated.

3.4.3 Sensitivity of the processes in the flushing months September 2003 and 2004

During each of the two regarded years, the main first flood events occurred in September, so for all variants, total flow and load were in more detail compared for these months in the years 2003 and 2004 for VSS, TSS and nitrate. In terms of flow, disregarding infiltration in scenario 2 caused an increase in total flow of 4% for September 2003 respective 43% for September 2004. Due to the lack of karstic flow in 09-2004, the total values for this month are significantly lower, so that transmission losses achieve greater importance.

	all	no trans- mission losses	no bacteria	no benthos	no fraction	double WWTP	no WWTP	no delivery	no karst	no quality	variable delivery WQ
VSS (S) [t/month] 09-2003	14.02	12.64	12.28	13.84	13.89	16.16	11.90	13.69	3.97	13.75	14.30
VSS (S) [%] 09-2003	100%	90%	88%	99%	99%	115%	85%	98%	28%	98%	102%
VSS (S) [t/month] 09-2004	5.68	4.20	4.60	5.32	5.15	10.01	1.29	5.27	5.65	3.99	6.03
VSS (S) [%] 09-2004	100%	74%	81%	94%	91%	176%	23%	93%	99%	70%	106%

Table 2: Loads of VSS for September 2003 and 2004 at site S, total values and percentages in terms of scenario 1

As result of the flow increase in scenario 2, the load of VSS is reduced by 10 to 26% (cp. Table 2). This is mainly caused by higher stream velocities and erosion. Bacteria are an important factor in the build-up of organic matter because up to 19% of VSS is caused by uptake of substrates (see 09-2004, "no bacteria"), but the benthic bacteria growth only accounts for 1 to 6%.

Transport and build up of VSS is strongly influenced by the biota. If all constituents in the simulation are considered to be conservative (scenario "no quality"), the total VSS flux is reduced by 30% in September 2004. So, the minor the input from the karst, the mayor the influence of the biological conversion processes become. If the karst is dominating, the built up organic matter is neglectable (2% in September 2003). If the substrate of the heterotrophic bacteria is doubled in concentration in the WWTP inputs, then the total load can be increased by 76%. Here, the influence of the karstic spring is once again more obvious, as it does not allow a proper accumulation instream in September 2003: the effect of higher organic substrate concentrations is much lower than in the year 2004, where there is hardly flow coming from site K. The situation is reversed in the variant without substrate inflow by the WWTPs (scenario 7, "no WWTP"), because here the additional loading of the spring becomes dominant and not, as in the case before, the additional erosion (and with it a reduction of accumulation potential) caused by the spring flow.

In the simulation, the delivery part of the model only accounts for 2 to 7% of VSS flow, whereas, if the karstic input of particulates and solubles is turned off, VSS is reduced by 72% for September 2003. The last variant with changing input concentrations for the delivery model did not yield major changes in total, but slightly increased the loadings. The changes in results for TSS are not so numerous as for VSS (see Table 3).

Table 3: Loads of TSS for September 2003 and 2004 at site S, total values and percentages in terms of scenario 1

	all	no trans- mission losses	no bacteria	no benthos	no fraction	double WWTP	no WWTP	no delivery	no karst	no quality	variable delivery WQ
TSS (S) [t/month] 09-2003	297.64	291.91	295.90	297.46	357.20	299.82	286.59	212.14	98.94	283.58	297.93
TSS (S) [%] 09-2003	100%	98%	99%	100%	120%	101%	96%	71%	33%	95%	100%
TSS (S) [t/month] 09-2004	69.57	69.22	68.50	69.21	73.38	73.86	64.58	14.39	62.56	63.93	69.93
TSS (S) [%] 09-2004	100%	99%	98%	99%	105%	106%	93%	21%	90%	92%	101%

Major variations are caused by the new fractional sediment transport approach. The total load of TSS is increased by 20% for the year 2003. If only the finest fraction is transported in the approaches with fractioned sediment, the total net erosion capacity is reduced in comparison to the approach without fractioned sediment, because the availability of the fine fraction on the river bed is limited due to the other two fractions (see EQ. 2-3). The interpretation of this is that some finer sediment is not mobilised because it is held in the interstices between immobile coarser material, i.e. that there is a hiding ability of the finer sediment fractions (see also e.g. Wu et al. (2000)).

In the comparison of variants "double WWTP" and "no quality" the influence of VSS on TSS can be estimated as between 1 and 8%.

The most significant influences are attributable to the karstic spring at K as well as for the delivery model. Which one prevails depends on the flow regime. If it is dominated by the spring, as in 09-2003, the TSS load is reduced by 2/3, if the karst concentration is set to zero. On the other hand, if the delivery model dominates the influence on the TSS load can be 79%.

However, the variations not only influence loadings of particulates. Table 4 shows nitrate loads, and it can be seen that during seasons of small flow volume, $\sim 60\%$ of the nitrate may be lost to the groundwater due to infiltration.

Table 4: Loads of NO3-N for September 2003 and 200	4 at site S, total values and percentages for scenario 1
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	all	no trans- mission losses	no bacteria	no benthos	no fraction	double WWTP	no WWTP	no delivery	no karst	no quality	variable delivery WQ
NO3-N (S) [kg/month] 09-2003	2 310	2 439	2 311	2 310	2 310	2 310	2 290	2 272	62	2 312	2 313
NO3-N (S) [%] 09-2003	100%	106%	100%	100%	100%	100%	99%	98%	3%	100%	100%
NO3-N (S) [t/month] 09-2004	53.24	84.15	53.38	53.25	53.24	53.24	49.88	4.43	52.88	53.38	54.86
NO3-N (S) [%] 09-2004	100%	158%	100%	100%	100%	100%	94%	8%	99%	100%	103%

The WWTP play a minor role in the nitrate transport in the catchment, only 1 to 6% of the total load can be assigned to the WWTP at site d. The karstic spring at the top of the catchment contributes most of the nitrate in the stream, up to 97% in September 2003.

3.4.4 NCL-plots for all scenarios

For TSS there is a good correspondence with the NCL-plot derived from the measurements (see Figure 7), the FF_{25} is about 65% for all variants.



Figure 7: Comparison of normalized cumulative loads of measured TSS and all scenarios at S for 2003.09-22

The simulation for VSS shows some deviations in comparison to the measurements. The flush occurs earlier in most of the scenarios, except in the variant without WWTP inflows and consideration of conversion processes ("without quality"). However, it is possible that the interval of the measurements at the very beginning of the flood is too long. The gradient of the measured curve matches the ones from the simulations at the beginning of the flood.



Figure 8: Comparison of normalized cumulative loads of measured VSS and all scenarios at S for 2003.09-22

As before for TSS, it can be seen that the karstic spring at K attenuates the first flush. Obviously, if the karst is considered to contain only perfectly clean water, as it is the case in scenario 9 ("no karst"), the load of the constituents will be zero at a later stage of the flood and the flush will be only caused by the amount of stored mass in the system prior to the event.



Figure 9: Comparison of normalized cumulative loads of measured NO3-N and all scenario at S for 2003.09-22

Clearly the karstic spring heavily influences the nutrient transport in the catchment, especially for nitrates. Owing to the accuracy of the measurements at the spring which were input in the model, there is a strong agreement between the simulation and the sampled data (cp. Figure 9).

4 Summary and discussion

The herein presented work documents the experiences gained while enhancing and testing the applicability of a freely available state-of-the-art water quality model. The MOHID Water Modeling System and its relation to the tempQsim STREAM model have been briefly presented, as well as the later modifications evolved during the work at the European project tempQsim. These processes were identified to be of great influence on the dynamics of temporary waters and are often not included in other modeling software.

The analysis on basis the scenarios underlined the importance of the introduced processes and the model's ability to simulate temporary rivers was demonstrated. In terms of annual or monthly loadings, the model shows a regular accuracy which is comparable to other available models. It is possible to model first flush loads caused by resuspension and biomass accumulation as well as the annual variation of the instream quality dynamics.

Although there could be presented important improvements on the instream parts, there still are mayor uncertainties in the parts concerning overland runoff. The remaining deviations seem to be mainly caused by missing information on the land side delivery of constituents.

Unfortunately, not only the knowledge on the hydrology, but also on the land side nutrient export is still very limited. Upscaling of the processes determined in laboratories is often not possible.

The application of the model at the catchment of the Vène showed some important issues concerning the calibration of temporary waters. The fluctuation of many system parameters have a greater and very important influence than in humid conditions.

Hence, future studies should focus on a better representation of the delivery part of models as well as a development of measures to account for the changing system parameters in calibration.

Acknowledgements

This study was founded by the European Commission under the contract number EVK1-CT2002-00112 and by the German Academic Exchange Service (DAAD).

The author wants to thank Ramiro Neves, Frank Braunschweig and Pedro Chambel Leitão (Instituto Superior Técnico (IST) at the Technical University of Lisbon) for their provision of the MOHID framework and the tempQsim consortium for the stimulating project work. Especially Marie-George Tournoud and Jean-Louis Perrin from the Maison de Science de L'Eau in Montpellier are acknowledged for the collection and provision of the intensive measured data and the simulations of MERCEDES.

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