



Modelling of a water filtration pilot by a chemical tracer using the Modflow "Finite Differences"

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ABSTRACT: For the supply of drinking water to the population, we have set up a surface water treatment system: horizontal sand filtration. This process is based on the principle of bank filtration; it is a natural rustic treatment, based on slow biological filtration, which does not require any reagent. The objective of this work is to propose a tool to describe the groundwater flow on a complete water filtration system with the MODFLOW model in order to follow the evolution of the hydrodynamic parameters on the one hand and to determine the transit time of the water in the pilot. The calibration with a chemical tracer, fluorescein, allowing to optimise the defined parameters (hydraulic conductivities, recharge) of the aquifer in order to obtain calculated loads as close as possible to those measured in given observation points, and the reading and saving of the imposed hydraulic loads were carried out with the "results extractor" module. The variation of the slope of the 2nd compartment from 5% to 20% significantly reduces the transit time of the tracer from 6.3 h to 5.2 h in the device. It was also found that the transit time increased as the sand grain size decreased, but this did not indicate a malfunction of the device. The results obtained showed that it is possible to perform a hydrodynamic modelling of the system in order to reproduce the experiments performed on the physical device. The steady-state modelling shows that the curves calculated at each piezometer are close to the experimental curves, except for the variation in sand grain size (piezometer 3), probably due to the preferred path. The differences in concentration between the calculated and experimental values at piezometers 3 and 4 are due to a dilution and/or adsorption effect by the fine sand. The calibration of the model allows an appropriate sizing according to each problem.

Keywords: Piezometer, Modelling, MODFLOW, MT3DMS, Tracert.

INTRODUCTION

A model is a tool for simulating reality. There are physical models such as laboratory and/or field tests and experiments and mathematical models that simulate groundwater flow indirectly by solving equations representing the physical processes occurring in the system as well as equations describing the boundary and initial conditions (Anderson and Woessner, 1992). The mathematical models can be solved analytically or numerically, and the analytical solutions have been established for controlled conditions, initial conditions, and simple boundaries (Anderson and Woessner, 1992). Indeed, groundwater during the replenishment of reserves related to precipitation, can be subjected to more or less turbid floods. The Modflow code (version 3.0) is a three-dimensional digital model. It describes groundwater flow in anisotropic and heterogeneous porous media, under stationary or transient flow conditions.

The Modflow software solves the partial differential diffusivity equation for groundwater flow in porous, anisotropic, and heterogeneous media under stationary or transient flow conditions for confined, free, or mixed aquifers (combination of Darcy's law and the continuity equation) by the finite difference method. To do this, the space is discretised in a cartesian system according to a rectangular mesh at the nodes of which the equation is solved. The PMWIN 5 processor (Processing Modflow for Windows; Chiang and Kinzelbach, 2001) was used to easily format the input data required for the model (geometry, boundary conditions, etc.) and

then to visualise the outputs of the modeling (hydraulic loads, concentration curves, etc.). The "PMPATH (Pathlines and Contours)" module of PMWIN5 retrieves the flow model created by the MODFLOW software and allows a graphic representation of the model. A model's purpose is to represent an entity or a real process schematically to understand and explain its operation and predict its behavior. The resultant extractor module was used to calibrate the aquifer using a tracer to optimise the defined parameters (hydraulic conductivity, recharge) in order to obtain calculated loads as close as possible to those measured at given observation points and to read and save the imposed hydraulic loads. Finally, the MT3DMS module was used to calculate hydrochemical parameters such as the evolution of the tracer concentration at different points of the device as a function of time. The objective of this work is to propose a tool for describing groundwater flow using a model.

This software uses the finite difference method for three-dimensional aquifer systems. The applications of this model related to the project are:

- (1) to figure out where the free surface of the groundwater table is at different times when different recharge conditions have been put into place over time,
- (2) to calculate the velocity and directions of groundwater flow and to evaluate the inflow (recharge) and outflow (breccia flow and seepage to groundwater) for these same periods.

MATERIALS AND METHODS

Experimental dispositif

For the application of the model, a horizontal flow filter pilot was constructed with a cross-section of 1 m^2 and a length of 14 m. It consists of the following elements (Figure 1). In hydrogeology, modelling is applied to transcribe, with the help of computer programming, the groundwater flow and the migration of the solute in the considered system. The first step in finite difference modelling is the discretisation of the model into a Cartesian system by a rectangular mesh of cells organised into rows (i), columns (j) and geological layers (k). Each layer represents an aquifer. Then, the diffusivity equation is solved at the mesh nodes by successive iterations based on the principle of flow continuity, where the difference between the inflow and outflow of the cell must be equal to the variation of the quantity stored in the cell as a function of time. The "MODFLOW finite difference" code, developed in Fortran by the USGS (Mc Donald and Harbaugh, 1996), was used to model the horizontal flow filtration device. We chose this software for its primary qualities of being simple, modular and having been made reliable through extensive use. The Modflow software solves the partial differential diffusivity equation for groundwater flow in porous, anisotropic and heterogeneous media at stationary or transient flow conditions for confined, free or mixed aquifers (combination of Darcy's law and the continuity equation) by the finite difference method. For this purpose, the space is discretised in a Cartesian system according to rectangular mesh at the nodes of which the equation is solved. The PMWIN 5 processor (Chiang and Kinzelbach, 2001) was used to easily format the input data required for the model (geometry, boundary conditions, etc.) and then to visualise the modelling outputs (hydraulic loads, concentration curves, etc.). The "PMPATH (Pathlines and Contours)" module in PMWIN5 retrieves the flow model created by the MODFLOW software and allows graphical representation of the model.

Model geometry and boundary conditions

In order to define the conditions of use of the MODFLOW model, the first step is to represent the exploitable surface of the device. The mesh adopted in this case is rectangular. The discretisation of the domain constitutes the step allowing to take into account the system's geometry and limits in the flow model. The pilot (14 m total length) was divided into 20 consecutive columns of 0.5 m width and 1 m height made up of materials of varying grain size (Figure 1):

- 6 columns of sand with a grain size of between 4 and 8 mm. The slope is 1%.
- 12 columns of sand with a grain size of 0 to 4 mm. The slope is 14%.
- 3 columns of gravel with a grain size of 20 to 40 mm. The slope is zero.

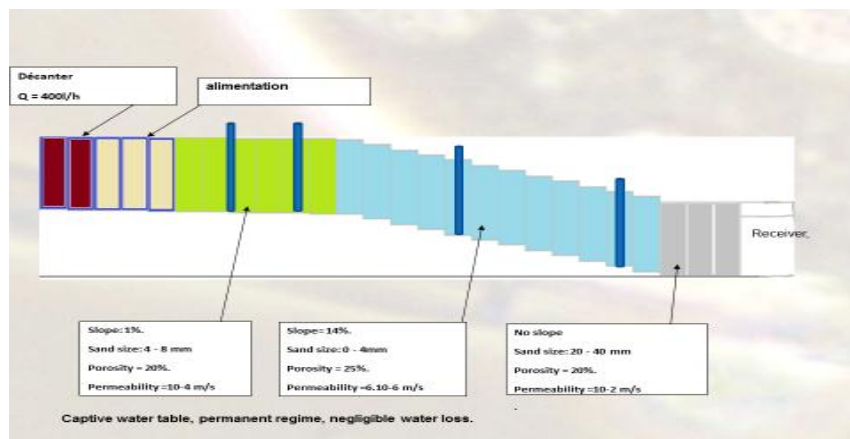


Fig. 1: View of the system in MT3DS

The simulation of the hydrodynamic behaviour of the aquifer is based on a rigorous definition of the boundary conditions. The role of these conditions is to impose on the aquifer in question the exchanges that condition its flow. In fact, the boundary conditions for the numerical model inherit the hypotheses that can be formulated from field observations (Louche B., 1997). Three types of boundaries have been proposed:

- imposed potential limit, the water level in the device is kept constant
- zero flow limit, only the water arrival is taken into account (no perpendicular flow takes place)
- At the imposed flow limit, infiltration is considered to be zero.

The second step consisted in defining the site's upstream and downstream boundary conditions as IBOUND (MODFLOW) imposed load boundaries for the flow models and ICBUND (MT3D) for the transport models. Indeed, the role of these boundary conditions is to impose on the aquifer the exchanges that condition its flow. As the device is neither exposed to light nor the open air, the water level is constant everywhere, so it is considered a saturated confined aquifer operating in a steady state. Furthermore, the medium is considered to be isotropic because the materials have identical properties in all directions. Finally, the altitude of the layered roof and the layered wall were calculated according to the terrain type.

2.2 Choice of model

In order to follow the evolution of the dye concentration on the one hand, and to determine the transit time of the water in the pilot, on the other hand, a numerical model was created. The calibration of the model makes it possible to identify the non-measured data by adjusting the calculated concentrations to the measured concentrations. Once the model has been calibrated, it can be used as a management and forecasting tool, making the pilot flexible. These tests consist of voluntarily incorporating a substance (artificial tracer) into the fluid under study, and they make it possible to describe either its movements or the physical, chemical or biological processes that it undergoes or that the compounds it contains undergo (Smart, P.L., and I.M.S. Laidlaw. 1997).

In the choice of the modelling tool the following assumptions were proposed:

Analysis in a steady or transient regime. Depending on the duration of the planned simulations and the importance of the slick fluctuations, a number of model dimensions were chosen: 1D, 2D vertical, 2D horizontal, quasi-3D, 3D; domain boundary conditions for flow and transport; initial conditions in the domain; homogeneity/heterogeneity, isotropy/anisotropy; number and type of phases; different chemical compounds involved; transport mechanisms in the domain; possibilities for exchange of chemical compounds between adjoining phases; chemical and physical or biological processes.

2.3 Choice and quantity of tracer to be injected

Tracers are increasingly used both to delimit the supply areas of water points, whether or not they are tapped, and the transit times of water and to simulate pollution. In hydrogeology, the tracer must be representative of the movement of water, i.e. its flow behaviour must be close to that of the water itself. For this, the following properties are required :

- Chemical stability ;
- Good solubility in water;
- Lowest possible adsorption tendency.

In addition, there are some important practical requirements:

- Safe for humans, animals and plants;
- Low detection limit;
- Low cost;
- Easy to quantify;
- No or low pollution load for the water.
- Natural concentration in the traced fluid.

Estimating the amount of tracer to be injected is an important preliminary step for a successful tracer test. The following formula is proposed to determine the amount of tracer needed for a tracing length L (Wernli, 1994; Kass, 1998; Goldscheider and Drew, 2007):

$$M = a \times L \times A,$$

- **M**: mass injected (g)
- **a** : tracer correction factor (g/m)
- **L**: distance (m)
- **A**: adjustment factor to aquifer conditions at permeability K
- $K > 10^{-3}$ m/s, $A = 0.25 \times$ aquifer thickness;
- $10^{-4} < K < 10^{-3}$ m/s, $A = 0.5 \times$ aquifer thickness;
- $K < 10^{-4}$ m/s, $A =$ aquifer thickness, m.

For fluorescein, $A=h= 1$, $L= 10$ metres representing the distance from the tracer injection point to the water outlet in the receiver.

$$M= 1 \times 10 \times 1 = 10 \text{ g.}$$

2.4 Model calibration

The calibration process consists of adjusting the calculated state to the actual (observed) form by modifying (adjusting) the values introduced for both the hydrodynamic parameters as well as those of the hypotheses made (Béranger et al., 2006). However, the hydrodynamic parameters determined from the experiments cannot vary. The same applies to the water flow rate entering the system. The spatial discretisation of the domain is the step that allows taking into account spatial discretisation of the domain, which allows the geometry and the limits of the system to be taken into account in the flow model. For this purpose, we have used the experimental data of fluorescein tracing as a function of time in each time in each compartment of the horizontal flow filtration device operating as a confined water table. Tracer tests are particularly well suited to characterise flows and complement the methods used in hydrogeology. They allow the nature of the groundwater flow to be understood and provide information on the physical structure and functioning of and functioning of the aquifer (Meus, 1993; Morales et al., 1995; Hauns et al., 2001). The basic idea of tracing techniques is to mark the water with a tracer, which makes it possible to follow its evolution in the environment. For each mesh, the initial hydraulic potential defined from the hydrodynamic data of the domain is constant. Therefore, the hydrodynamic data of the domain is constant. The water level is assumed to be stable in the steady-state hydraulic regime. Therefore, the water level in each compartment is assumed to be stable. The variation in the volume of water stored in a porous medium is zero, so the inflow is equal to the outflow. When the calculations seem correct, it is necessary to verify this hypothesis because the model allows for this hypothesis, as the model allows access to the water budget module to validate the calibration.

2.5 Calibration check

Such a test aims to observe an entity's spatial and temporal evolution within the pilot. Its evolution is observed over time at several locations using the observation piezometers installed on the device (Table I). To validate our model, we used the data obtained (observed) during the fluorescein tracing ($C_{20}H_{10}Na_2O_5$ or 3H-xanthene-3-on) to determine the transit time of the water in the pilot. First, all the hydrodynamic parameters necessary for the operation of the model were introduced (effective porosity, horizontal hydraulic conductivity, inlet flow rate, and hydraulic load). Then, the determination of the water level in each compartment of the device as well as the concentration of fluorescein as a function of time is carried out. The measurement points concern the decanted water tank (ED), the water at the filter outlet (EF) and the four piezometers used as sampling points. The MT3DMS module calculates the tracer concentration as a function of its spatial and temporal evolution. The dispersion coefficient was simulated to obtain an approximate response between the calculated and observed values. This step minimises the difference between the measurements and the results, by adjusting the input data until the model reproduces the conditions of the measured field with an acceptable level of accuracy. The dispersion coefficient is proportional to the average flow velocity of water in the pores, and represents the medium's inherent characteristics, depending, among other things on its heterogeneity. Its value for this response is 10^{-13} . The adsorbed phase's molecular diffusion coefficient values are $< 10^{-12}$ (Raoul Calvet, 2003). This value gave the best restitution of the model in steady state. This calibration was carried out manually. Ideally, the model should be validated on data not used during calibration to test its predictive ability (Béranger S., Guérin V., Picot G. 2006). Table 1 shows the coordinates of the water sampling points for the determination of tracer concentrations as a function of time.

Table 1: Coordinates of monitoring points

No.	Borehole Name	Active	X (easting)	Y (northing)	Layer
1	ED	<input checked="" type="checkbox"/>	2,05	0,5	1
2	P1	<input checked="" type="checkbox"/>	3,97	0,5	1
3	P2	<input checked="" type="checkbox"/>	5,37	0,5	1
4	P3	<input checked="" type="checkbox"/>	8,12	0,5	1
5	P4	<input checked="" type="checkbox"/>	10,47	0,5	1
6	EF	<input checked="" type="checkbox"/>	13,25	0,5	1
7	EB	<input checked="" type="checkbox"/>	0,52	0,5	1

RESULTS AND DISCUSSION

Sensitivity analysis

Sensitivity analysis of a model can be carried out by varying one or more parameters strongly. In this study, two parameters were chosen to test the model's sensitivity to their variation. The sensitivity tests concern the following parameters: the porosity and the molecular dispersion coefficients, as the other coefficients were determined experimentally. The objective is to determine the influence of a particular parameter on the response of the model. The analysis of the concentration curves shows a significant variation when changing the values of effective porosity and the molecular dispersion coefficient.

Comparison of Calculated and Observed Curves

Normal Gaussian distribution

Figure 2 shows the overall evolution of the fluorescein concentration as a function of time determined experimentally and calculated with the model.

Then, we tried to repeat the representation in each monitoring point this time, as shown in figures 3 a, b, c, d, e and f.

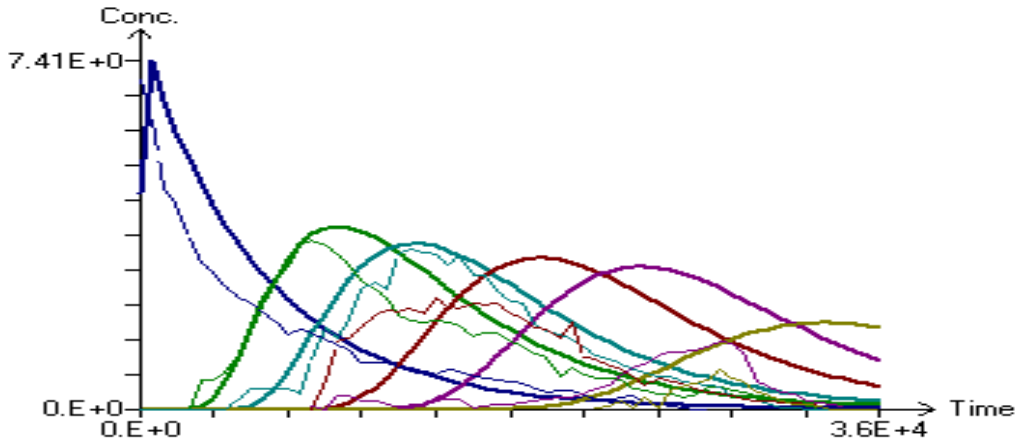


Fig. 2: Overview of each piezometer's experimentally observed (dotted) and calculated (bold) curves. Concentration: mg/l and time in seconds (s).

Figures 3 show the evolution of the observed and calculated curves in each pilot compartment.

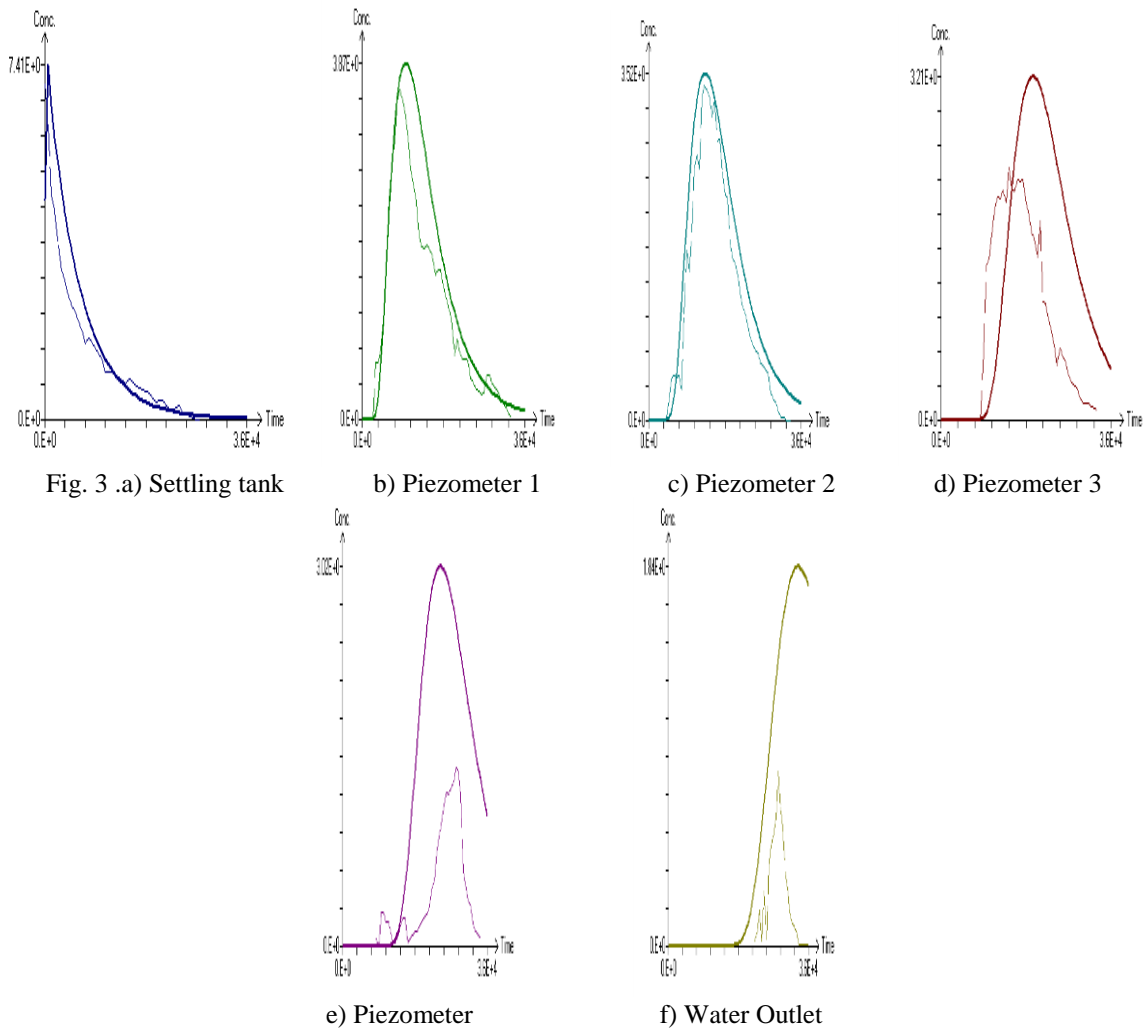


Figure 3 : Comparison of the calculated (bold line) and observed curves as a function of time in the water at each point (Piezometers 1, 2, 3 and 4, Settling tank (before entry) and filtered water (at exit)).

Interpretations

The calibration of the model has allowed for the representation of the evolution in time of the concentrations of the tracer used. We note a shift on the third piezometer between the curves of the calculated and observed values in the field. The responses of piezometers 1 and 2, as well as those of the decanted water (ED), are in accordance with the expectations of the model. The shift of the observed and calculated curves at piezometer 3 may be due to a preferential passage of water in the filtration device because it is located in the zone constituted by the division of the 2 materials of granulometry (4-8 mm and 0-4 mm) and in the zone of the strong slope, with speed increasing because of the lower granulometry. In an ideal case, the artificial tracer should be completely absent from the traced fluid in order to follow its restitution unambiguously. Otherwise, its natural content should be low compared to the concentrations of the returned fluids. As the number of observation points in space is limited, it is logical to try to extract as much information as possible about the movement of the tracer cloud from its temporal variations at the different output points. The difference in concentration between the experimental and calculated values increases from piezometer 3 onwards, from the finest sands onwards. (Zahn and Behrens ,1992) It highlighted fluorescein adsorption in a glacial gravel aquifer by conducting tests with various tracer concentrations. Indeed, they observe a delay factor of fluorescein about chloride and bromide ions which is all the more important as the injected fluorescein content is low.

Water balance in the system

The water balance allows us to assess the case of a possible failure in the system, e.g. water leakage from the system. The results obtained in the table below show simulation results with a balanced input-output balance and a rapid convergence of the model. It was also found that the inflow and outflow are of the same order of magnitude ($1.1 \cdot 10^{-4} \text{ m}^3/\text{s}$), with a difference of $1.891 \cdot 10^{-10}$ representing the water loss in the device (Table 2).

Table 2: Water balance at the inlet and outlet of the device.

FLOW TERM	IN	OUT	IN-OUT
STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
CONSTANT HEAD	1.1000019E-04	0.0000000E+00	1.1000019E-04
WELLS	0.0000000E+00	1.1000000E-04	-1.1000000E-04
DRAINS	0.0000000E+00	0.0000000E+00	0.0000000E+00
RECHARGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
ET	0.0000000E+00	0.0000000E+00	0.0000000E+00
RIVER LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
HEAD DEP BOUNDS	0.0000000E+00	0.0000000E+00	0.0000000E+00
STREAM LEAKAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
INTERBED STORAGE	0.0000000E+00	0.0000000E+00	0.0000000E+00
MULTI-AQIFR WELL	0.0000000E+00	0.0000000E+00	0.0000000E+00
SUM	1.1000019E-04	1.1000000E-04	1.8917490E-10
DISCREPANCY [%]	0.00		

Application of the model: Evolution of the water transit time after modification of the granulometry of the sand and the slopes in the first two compartments

Influence of the granulometry of the sand in the first compartment.

We have observed that fine particles pass through the geomembrane installed at the entrance of the sand bed with granulometry between 4 and 8 mm. It is assumed that after some time of operation of the filter, finer particles of size between 0 and 4 mm can successively occupy 0.5; 1; 1.5; 2 or even the entire 0 and 4 mm portion. The results in Table 3 below have enabled us to determine the transit time of the tracer as a function of the evolution of fine particles in metres in section 1 of the sand bed.

Table 3: Evolution of the water transit time after modification of the sand granulometry

Evolution of Fine Particles, mm	0,5	1	1,5	2	3
Transit time, h	5,6	5,6	5,7	5,8	6

It can be seen that the transit time increases when the granulometry of the sand decreases without, however, indicating a malfunction of the device.

Effect of the evolution of the slopes of the two compartments.

In this paragraph, we have evaluated the influence of the slopes of the two compartments on the water transit time to enable us to appreciate the Effect of this parameter. We have kept the total length of the pilot and the different compartments constant, a dimension imposed on us by the length of the land available to us.

We first varied the slope of the first compartment of length 3 m, a compartment composed of sand of granulometry included between 4 and 8 mm, then a second time to vary the second part, that composed of fine sand of granulometry 0 - 4 mm and length 5m. The results obtained are shown in tables 4 and 5.

Table 4. Influence of the Variation of the slope (%) of compartment 1

slope 1, %	Slope 2, %	Transit time, h
0,2	14	5,9
0,5	14	5,7
0,6	14	5,7
1	14	5,6
1,5	14	5,5
2	14	5,5
4	14	5,4
5	14	5,4

In the second step, we held the slope of compartment 1 constant and varied the slope of the second compartment. The results are shown in Table V.

Table 5: Influence of the Variation of the slope of the second compartment (percentage)

slope 1, %	slope 2, %	Transit time, h
1	5	6,30
1	8	6,00
1	10	5,80
1	12	5,70
1	14	5,60
1	15	5,60
1	18	5,20
1	20	5,20

The results in Tables 4 and 5 show that the water transit speed is, as expected, influenced by the slope of the two compartments. It can be seen that if the pitch of the first compartment is decreased or increased by a factor of 5, the transit time varies by 4 to 6%, whereas a smaller variation in the slope of the second compartment (60%) causes the transit time to vary by 12.5%. To better compare the influence of the slopes, we have plotted the evolution of the influence of the slopes of the two compartments on the transit time in Figures 5 and 6.

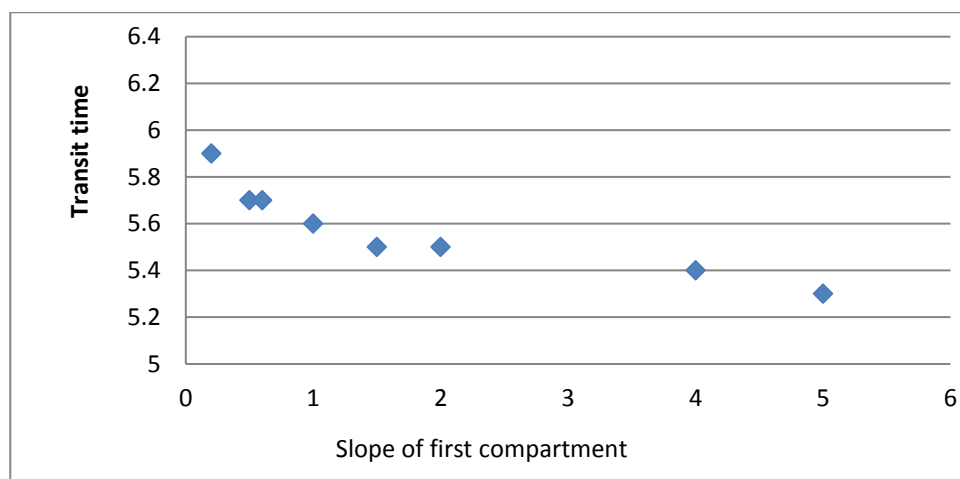


Figure 5: Influence of the slope of the first compartment (in percentage) on the transit time

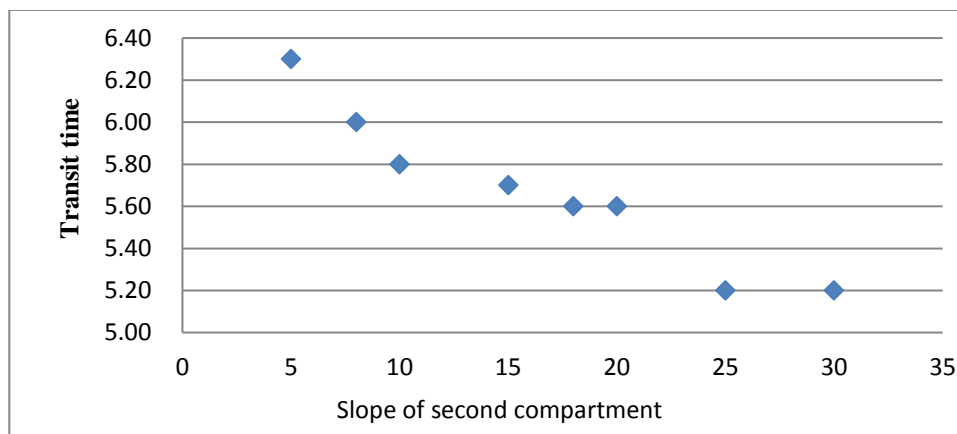


Figure 6: Influence of the slope of the second compartment (in percent) on the transit time.

Figure 5 shows that the variation of the slope of the first compartment has little influence on the transit time for values higher than 1%. This result shows that the slope we chose for our pilot was well chosen. On the contrary, the evolution of the transit time if the slope of the second compartment is modified decreases almost linearly with the slope increase. We can conclude that the second compartment's slope is the most important factor for varying the transit time. This result is important if we want to improve the purifying power of the filter in the case of slow degradation kinetics of bacteriological contaminants.

CONCLUSION

The use of artificial tracing to solve hydrological problems is being developed. The aim is to determine flow directions or velocities, residence times, or to represent a polluting substance's transport, dispersion or delay. The ideal tracer for each of these questions does not exist, and there is a great deal of research into the behaviour of tracers. The results have shown that it is possible to carry out hydrodynamic modelling of the system to reproduce the experiments carried out on the physical device. We have seen that a dynamic regime is established in the case of injection into a constant volume of water (due to the continuous feed into the decanter). The results of the steady state modelling show that the curves calculated at each piezometer are close to the experimental curves, except at the change of sand grain size (piezometer 3), probably due to the preferred path.

For now, it was impossible to figure out the differences between the calculated and measured concentrations at piezometers 3 and 4. However, we can suggest a dilution and/or adsorption effect from the fine sand. We propose that batch experiments be used to test this last hypothesis and determine the adsorption capacity of these sands towards fluorescein. We demonstrated using software that the slope of the second compartment significantly impacts the transit time of the water in the pilot. The calculated model can be used to simulate groundwater flow on a regional scale as well as aquifer-stream flows. Model sensitivity analysis was carried out on the MODFLOW model to identify the variables and parameters controlling the groundwater flow dynamics. The effect of variations in hydraulic conductivity and slope was studied. The hydraulic conductivity was reduced to 10% and increased to 1000% of its calibrated value. The model calibration allows the identification of unmeasured data by adjusting the calculated concentrations to the measured concentrations. The model, once calibrated, can be used as a management and forecasting tool, making the pilot scalable, and should subsequently enable the appropriate sizing of the pilot to be proposed, depending on the problem.

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Ethical Clearance Number

No applicable.

Competing Interests

No potential conflict of interest.

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Authors Contributions

All the authors contributed equally to this work.

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