

# Numerical Modeling and Simulation of the Transfer of Polluted Water by Pesticid in an Agricultural Area and Comparison of the Results with the PRZM and PEARL Models

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**Abstract-**Agricultural activity significantly modifies the quality and dynamics of water in the environment. By transforming the plant cover, working the soil, and adding fertilizer and pesticides, agriculture alters the cycle of water and its compounds. The quality of water around the world has deteriorated significantly in recent years, due to uncontrolled industrial discharges, the intensive use of pesticides and chemical fertilizers in agriculture as well as the disorderly exploitation of water resources. These produce a chemical modification of the water and make it unsuitable for the desired uses. the European directive which sets, for water intended for consumption, at  $0.1\mu\text{g/l}$  the maximum authorized concentration for each pesticide and at  $0.5\mu\text{g/l}$  that concerning the total pesticides. To fight water pollution by agricultural pesticides origin, Western countries have developed numerical models of pesticide transfer, the use of which remains very difficult in sub-Saharan Africa due to the insufficiency of the necessary data and parameters, however Agriculture represents the main activity of more than 80% of the population in sub-Saharan Africa. In this work, a new model for the flow of pesticide-laden water was developed. This model was compared in terms of performance to the PRZM and PEARL models on horizons of 0-20 cm, 20-50 cm, 50-100 cm and for time intervals of 10 min, 20 min, 30 min, 40 min, 50 mins, 60 mins, 70 mins and 80 mins. The performance of the developed model was respectively 0.95; 0.94 and 0.93 on the horizons of 0-20, 20-50 and 50-100 cm. Those of the PRZM model were respectively 0.96; 0.97 and 0.94 over the same horizons and those of the PEARL model were respectively 0.98; 0.98 and 0.97 over the same horizons. To better compare the performances of these different models, the RMSE and MAPE values were calculated for each model and for each horizon. The MAPE(%) values for the developed model were -2.17, respectively; -1.66 and -3.88 for the 0-20, 20-50 and 50-100 cm horizons and those of RMSE were  $4.13 \times 10^{-5}$  respectively;  $4.43 \times 10^{-6}$  and  $5.45 \times 10^{-6}$ . The MAPE(%) values for the PRZM model were -0.69, respectively; -0.49 and -2.81 for horizons 0-20, 20-50 and 50-100 cm and the RMSE values were  $1.36 \times 10^{-5}$ , respectively;  $1.96 \times 10^{-6}$  and  $3.54 \times 10^{-6}$  for the same horizons. The MAPE(%) values for the PEARL model were -0.33, respectively; -0.28 and -2.68 for the 0-20, 20-50 and 50-100 cm horizons while those of RMSE were respectively  $5.45 \times 10^{-6}$ ;  $3.54 \times 10^{-6}$  and  $1.47 \times 10^{-6}$ . The good performance of the developed model allows it to be used for simulating the transfer of water laden with pesticides in watersheds.

**Keywords:** Cameroon, model, simulation, infiltration, pesticides, pollution

## I. INTRODUCTION

To fight against pollution from the agricultural environment, it is important to know it well and quantify it, but above all to help farmers adopt appropriate land management techniques and good agricultural practices [1]. The use of a model to simulate the impact of management practices on the water quality of rivers constitutes a very important decision-making tool [2]. Assessing the risks associated with pesticides is a key step in preventing environmental contamination [3]. Indeed, the use of pesticides generates a certain number of risks with regard to the chemical composition of the air, water and soil which result in pollution whose toxicological and ecotoxicological consequences can be detrimental to environmental quality [4]. The world population is growing rapidly and by 2025, 52% of this population will live in urban areas [5]. Africa has the highest growth rate in the world estimated at 2.55% per year between 2010 and 2015. By 2050, Africa will represent a quarter of the world's population with an estimated population of 1.3 billion inhabitants [6]. In this work, a model for the transfer of water laden with pesticides was developed, this model was tested on the Djuttitsa watershed in western Cameroon and the results of the numerical simulations were compared to the results obtained with the models. PRZM and PEARL on the same horizons and at the same moments of time.

## II. MATERIALS AND METHODS

### A. Presentation of the study area

Djuttitsa is situated on the southern flank of the Bamboutos mountain in the Western Region of Cameroon [7] between latitude  $5^{\circ}24'$  and  $5^{\circ}45'$  North, and between longitude  $10^{\circ}2'$  and  $10^{\circ}40'$  (Figure 1). This area was selected due to the intensive agricultural activities carried out there, with high use of pesticides. The predominant crops cultivated are irish potatoes, cabbages, carottes, spices and tea [8].

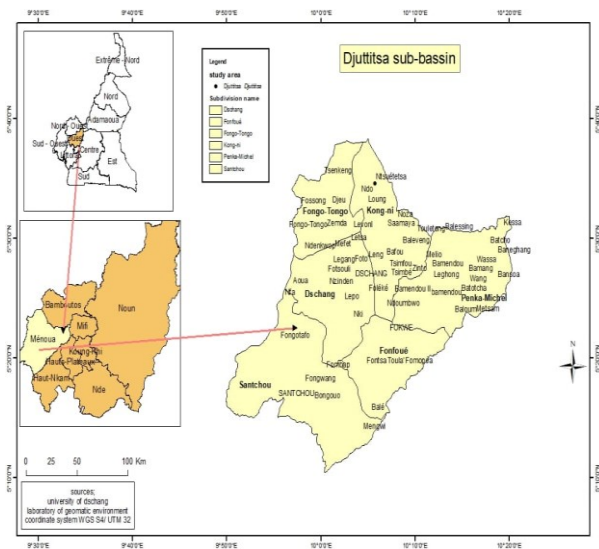


Figure 1: Location of the study area

In this study, a one dimension (1-D) mathematical model was developed to determine the movement of a pesticide from the soil surface to the depth of 1 m [9]. A depth of 1 m was used because at the study site, after a depth of 1 m, the soil properties were uniform. Paraquat (C<sub>12</sub>H<sub>14</sub>N<sub>2</sub>) a weed killer was selected for use. The 1 m depth was divided into 10 equal horizons of 10 cm each in order to have a constant space step in the mathematical model. The model was developed to simulate the concentration of paraquat at 10, 20, 30, 40, 50, 60, 70, 80, 90 and 100 cm depths as a function of time [10]. In the laboratory, an experiment was setup to determine the concentration of paraquat at the above mentioned depths. The comparison between values of concentrations obtained in the laboratory and those predicted by the model was used to validate the model [11].

B. Modeling of pollutant movement in the soil using the convection-dispersion equation

1.) The convection-dispersion equation

The development of a pesticide transfer numerical model necessitates the resolution of the convection-dispersion equation that controls the transport of pollutants in the soil [12] :

$$\begin{cases} \frac{\partial}{\partial t} [R(\theta)C] - \frac{\partial}{\partial z} \left[ D(\theta, v) \frac{\partial C}{\partial z} \right] + \frac{\partial}{\partial z} [vC] = 0 \text{ in } ]0, 1[ \\ C(z, 0) = C_0(z) \\ C(0, t) = c(1, t) = 0 \end{cases} \quad (1)$$

$$R(\theta) = 1 + \rho \frac{K_d}{\theta} \quad (2)$$

C, pollutant concentration in the soil in mol.l<sup>-1</sup>

K<sub>d</sub>, transfer coefficient between solid and liquid phase

D, dispersion coefficient

ρ, soil density

θ, water content in g.(cm<sup>3</sup>)<sup>-1</sup>

C<sub>0</sub> is the initial concentration in mol.l<sup>-1</sup>

2.) Richards Equation

The Richards equation which governs the flow of water in the ground is written [13]:

$$\begin{cases} C(h) \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} [K(h) \left( \frac{\partial h}{\partial z} - 1 \right)] \\ h(0, z) = h_{ini}(z) \\ h(t, 0) = h_{surf}(z) \\ h(t, Z) = h_{fond}(z) \end{cases} \quad (3)$$

Where K is the hydraulic conductivity: it accounts for the ability of the porous medium to transmit the water it contains for a given water content.

h is the relative pressure compared to the atmospheric pressure of the water expressed as water height.

Z is the vertical axis positively oriented downward.

Solving this Richards equation in an unsaturated zone requires knowledge of two other hydrodynamic functions: the functions C(h) and K(h)

The functions C(h) and K(h) are defined empirically by [14]

$$C(h) \begin{cases} \frac{\theta_s(2-n)}{h_g} \left( \frac{h}{h_g} \right)^{n-1} \left[ 1 + \left( \frac{h}{h_g} \right)^n \right]^{\frac{2}{n}-2}, & si \ h < 0 \\ 0, & si \ h \geq 0 \text{ (cas saturé)} \end{cases} \quad (4)$$

$$K(h) \begin{cases} K_s \left[ 1 + \left( \frac{h}{h_g} \right)^n \right]^{m \left( \frac{2}{n}-1 \right)}, & si \ h < 0 \\ K_s, & si \ h \geq 0 \text{ (cas saturé)} \end{cases} \quad (5)$$

The different parameters designate respectively:

θ<sub>s</sub> the water content at natural saturation,

K<sub>s</sub> the hydraulic conductivity at saturation,

m and n the parameters linked to the structure of the soil,

h<sub>g</sub> the inflection point of the retention curve h=f(θ) defined by:

$$f(x) = \theta_s \left[ 1 + \left( \frac{x}{h_g} \right)^n \right]^{\frac{2}{n}-1} \quad (6)$$

These two equations were solved numerically by the finite volume method which is particularly suited to solving problems of conservation of matter.

C. Determination of experimental concentration in the laboratory

A paraquat solution was prepared with similar concentration to that used by farmers in the study area. That is, 75 ml of paraquat 200 mg.l<sup>-1</sup> in 15 l of water. This gave a concentration of 5ml for 1l, with a molar concentration of 5.4x10<sup>-4</sup> mol.l<sup>-1</sup>.

Soil samples were washed with water and the filtrate collected and analyzed under a UV-visible spectrophotometer to ensure the initial absence of paraquat in the soil.

Non polluted soil samples were collected in the study site using cylindrical rings of 10 cm height at different depth: 0-10, 10-20, 20-30, 30-40, 40-50, 50-60, 60-70, 70-80, 80-90, 90-100 cm. The filtrate was collected at 10 minutes interval. The absorbance of the solution was read at wavelength of 268 nm using a UV-visible spectrophotometer

D. Calculation of model efficiency

The performance of a model is its ability to reproduce the real environment with an acceptable margin of error. It was evaluated by calculating its effectiveness for each horizon according to the following formula according to Marin-Benito, [14].

$$EF = 1 - \frac{\sum_{i=1}^n (S_i - O_i)^2}{\sum_{i=1}^n (O_i - \bar{O})^2} \quad (7)$$

Where  $O_i$ : observed value  
 $\bar{O}$ : average of  $O_i$   
 $S_i$ : simulated value  
 $n$ : number of observations

The general performance was obtained by taking the arithmetic average of the performances of the different horizons [15].

III. RESULTS AND DISCUSSION

A. Numerical model

The numerical solutions of the Richards and convection-dispersion equation obtained numerically by the finite volume method are:

The Richards equation which governs the infiltration of water into the soil is as follows

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ D(\theta) \frac{\partial \theta}{\partial z} \right] - \frac{\partial D(\theta)}{\partial z} \quad \text{sur } [0, 1]$$

$$D(\theta) = \frac{K(\theta)}{C(\theta)}$$

$$C(h) = \frac{\theta_s(2-n)}{h_g} \left( \frac{h}{h_g} \right)^{n-1} \left[ 1 + \left( \frac{h}{h_g} \right)^n \right]^{\frac{2}{n}-2} \quad (8)$$

$$K_s \left[ 1 + \left( \frac{h}{h_g} \right)^n \right]^m \left( \frac{2}{n}-1 \right)$$

$$\theta(h) = \theta_r + (\theta_s - \theta_r) \left[ \frac{1}{1 + (\alpha h)^n} \right]^m$$

The finite volume method presented in the methodology made it possible to obtain the numerical scheme (9) for the numerical resolution of the Richards equation:

$$\frac{mes(\zeta_i)}{\Delta t} (\theta_{\zeta_i}^{n+1} - \theta_{\zeta_i}^n) = F_{i+\frac{1}{2}}^n - F_{i-\frac{1}{2}}^n \quad (9)$$

$$\text{où } F_{i+\frac{1}{2}}^n = \frac{2D_i^n D_{i+1}^n}{D_i^n + D_{i+1}^n} \frac{\theta_{i+1}^n - \theta_i^n}{\delta} - D_i^n$$

The convection-dispersion equation which governs the transport of pollutants in the soil and which has been solved numerically is as follows:

$$\left\{ \begin{aligned} \frac{\partial}{\partial t} [R(\theta)C] - \frac{\partial}{\partial z} \left[ D(\theta, v) \frac{\partial C}{\partial z} \right] + \frac{\partial}{\partial z} [vC] &= 0 \quad \text{dans } ]0, 1[ \\ C(z, 0) &= C_0(z) \\ C(0, t) &= c(1, t) = 0 \end{aligned} \right. \quad (10)$$

The numerical scheme obtained by the finite volume method for the numerical resolution of the convection-dispersion equation is given by system (10):

$$R_i^n h_i \frac{C_i^{n+1} - C_i^n}{k} + D_i^n \left( -\frac{C_{i+1}^n - C_i^n}{h_{i+\frac{1}{2}}} + \frac{C_i^n - C_{i-1}^n}{h_{i-\frac{1}{2}}} \right) + v(C_i^n - C_{i-1}^n) = 0$$

$$C_i^0 = \frac{1}{h_i} \int_{K_i} C_0(z) dz \quad \forall i = 1, \dots, N$$

$$C_0^n = C_{N+1}^n = 0$$

The numerical model which is a combination of numerical solutions of the convection-dispersion and Richards equations is written as follows:

$$R_i^n h_i \frac{C_i^{n+1} - C_i^n}{k} + D_i^n \left( -\frac{C_{i+1}^n - C_i^n}{h_{i+\frac{1}{2}}} + \frac{C_i^n - C_{i-1}^n}{h_{i-\frac{1}{2}}} \right) + v(C_i^n - C_{i-1}^n) = 0$$

$$\frac{mes(\zeta_i)}{\Delta t} (\theta_{\zeta_i}^{n+1} - \theta_{\zeta_i}^n) = F_{i+\frac{1}{2}}^n - F_{i-\frac{1}{2}}^n$$

$$C_i^0 = \frac{1}{h_i} \int_{K_i} C_0(z) dz \quad \forall i = 1, \dots, N$$

$$C_0^n = C_{N+1}^n = 0 \quad (12)$$

The graphical interface of the developed model is as follows:

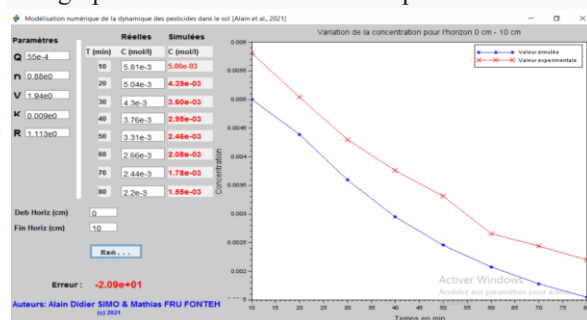


Figure 2: Graphical interface of the new developed model [16].

B. Comparison between the simulation values of the model developed with the PRZM and PEARL models

The values obtained by simulation with the new developed model were compared to the values obtained by simulation with the PRZM and PEARL models. These values were compared on the horizons 0-20 cm, 20-50 cm and 50-100 cm and on the time intervals of 10 min, 20 min, 30 min, 40 min,

50 min, 60 min, 70 min and 80 min flow. These comparisons were made with a table then with a diagram for each horizon.

1.) Comparison on the 0-20 cm horizon

Table 1 presents the results of the values simulated by the new model developed and the PRZM and PEARL models on the 0-20 cm horizon. These values are compared for the same instant of time.

Tableau1 : comparison between simulated values on the 0-20 cm horizon

Temps (min)	Concentrations observées (mol.l <sup>-1</sup> )	Nouveau modèle (mol.l <sup>-1</sup> )	PRZM (mol.l <sup>-1</sup> )	PEARL (mol.l <sup>-1</sup> )
10	5.6x10 <sup>-3</sup>	5.5x10 <sup>-3</sup>	5.6x10 <sup>-3</sup>	5.6x10 <sup>-3</sup>
20	3.6x10 <sup>-3</sup>	3.1x10 <sup>-3</sup>	3.5x10 <sup>-3</sup>	3.6x10 <sup>-3</sup>
30	1.9x10 <sup>-3</sup>	1.8x10 <sup>-3</sup>	2.0x10 <sup>-3</sup>	1.8x10 <sup>-3</sup>
40	1.71x10 <sup>-3</sup>	1.6x10 <sup>-3</sup>	1.7x10 <sup>-3</sup>	1.6x10 <sup>-3</sup>
50	1.1x10 <sup>-3</sup>	1.0x10 <sup>-3</sup>	1.1x10 <sup>-3</sup>	1.1x10 <sup>-3</sup>
60	7.4x10 <sup>-4</sup>	7.3x10 <sup>-4</sup>	7.3x10 <sup>-4</sup>	7.4x10 <sup>-4</sup>
70	5.5x10 <sup>-4</sup>	5.3x10 <sup>-4</sup>	5.4x10 <sup>-4</sup>	5.5x10 <sup>-4</sup>
80	4.1x10 <sup>-4</sup>	4.0x10 <sup>-4</sup>	4.0x10 <sup>-4</sup>	4.1x10 <sup>-4</sup>

Figure 3 illustrates the simulation points on the 0-20 cm horizon between the new model and the PRZM and PEARL models. These simulation points are made at the same instants of time

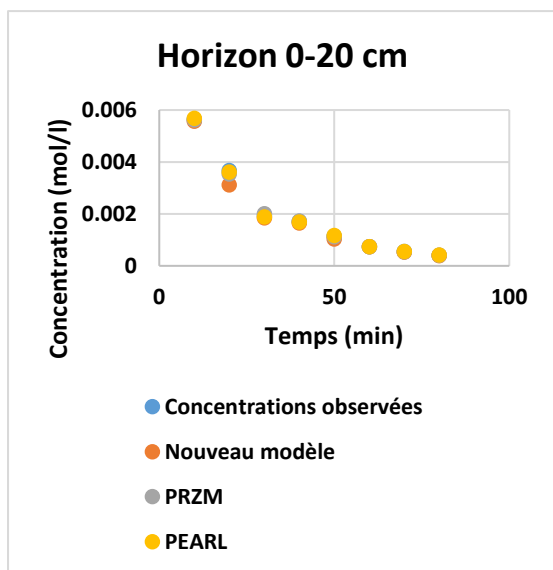


Figure 3: Comparison of simulation points between the new model and the PRZM and PEARL models on the 0-20 cm horizon

2.) Comparison on the 20-50 cm horizon

Table 2 presents the results of the values simulated by the new model developed and the PRZM and PEARL models over the 20-50 cm horizon. These values are compared for the same instant of time.

Tableau2 : Comparison between simulated values on the 20-50 cm horizon

Temps (min)	Concentrations observées	Nouveau modèle (mol.l <sup>-1</sup> )	PRZM (mol.l <sup>-1</sup> )	PEARL (mol.l <sup>-1</sup> )
10	4.2x10 <sup>-3</sup>	4.1x10 <sup>-3</sup>	4.2x10 <sup>-3</sup>	4.2x10 <sup>-3</sup>
20	1.6x10 <sup>-3</sup>	1.5x10 <sup>-3</sup>	1.6x10 <sup>-3</sup>	1.6x10 <sup>-3</sup>
30	5.2x10 <sup>-4</sup>	5.1x10 <sup>-4</sup>	5.2x10 <sup>-4</sup>	5.2x10 <sup>-4</sup>
40	2.4x10 <sup>-4</sup>	2.3x10 <sup>-4</sup>	2.4x10 <sup>-4</sup>	2.4x10 <sup>-4</sup>
50	9.3x10 <sup>-5</sup>	9.2x10 <sup>-5</sup>	9.2x10 <sup>-5</sup>	9.2x10 <sup>-5</sup>
60	4.0x10 <sup>-5</sup>	3.9x10 <sup>-5</sup>	3.9x10 <sup>-5</sup>	4.0x10 <sup>-5</sup>
70	1.8x10 <sup>-5</sup>	1.8x10 <sup>-5</sup>	1.8x10 <sup>-5</sup>	1.9x10 <sup>-5</sup>
80	9.0x10 <sup>-6</sup>	8.9x10 <sup>-6</sup>	8.93x10 <sup>-6</sup>	8.98x10 <sup>-6</sup>

Figure 4 illustrates the simulation points on the 20-50 cm horizon between the new model and the PRZM and PEARL models. These simulation points are made at the same instants of time

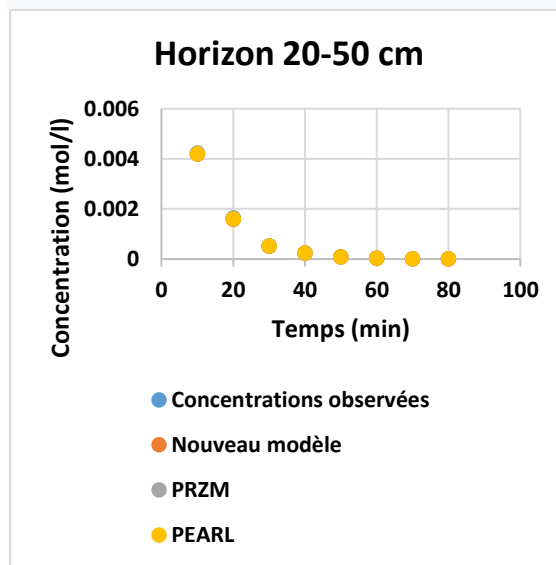


Figure 4: Comparison of simulation points between the new model and the PRZM and PEARL models on the 20-50 cm horizon

3.) Comparison on the 50-100 cm horizon

Table 3 presents the results of the values simulated by the new model developed and the PRZM and PEARL models over the 50-100 cm horizon. These values are compared for the same instant of time.

Tableau 3 : Comparison between simulated values on the 50-100 cm horizon

Temps (min)	Concentrations observées	Nouveau modèle (mol.l <sup>-1</sup> )	PRZM (mol.l <sup>-1</sup> )	PEARL (mol.l <sup>-1</sup> )
10	2.7x10 <sup>-3</sup>	2.6x10 <sup>-3</sup>	2.6x10 <sup>-3</sup>	2.6x10 <sup>-3</sup>
20	5.2x10 <sup>-4</sup>	5.1x10 <sup>-4</sup>	5.1x10 <sup>-4</sup>	5.2x10 <sup>-4</sup>
30	6.2x10 <sup>-5</sup>	6.1x10 <sup>-5</sup>	6.2x10 <sup>-5</sup>	6.1x10 <sup>-5</sup>
40	1.1x10 <sup>-5</sup>	1.0x10 <sup>-5</sup>	1.2x10 <sup>-5</sup>	1.3x10 <sup>-5</sup>
50	1.8x10 <sup>-6</sup>	1.6x10 <sup>-6</sup>	1.7x10 <sup>-6</sup>	1.7x10 <sup>-6</sup>
60	3.0x10 <sup>-7</sup>	3.0x10 <sup>-7</sup>	3.7x10 <sup>-7</sup>	2.9x10 <sup>-7</sup>
70	6.5x10 <sup>-8</sup>	6.4x10 <sup>-8</sup>	6.5x10 <sup>-8</sup>	6.7x10 <sup>-8</sup>
80	1.6x10 <sup>-8</sup>	1.5x10 <sup>-8</sup>	1.62x10 <sup>-8</sup>	1.60x10 <sup>-8</sup>

Figure 5 illustrates the simulation points on the 50-100 cm horizon between the new model and the PRZM and PEARL models. These simulation points are made at the same instants of time

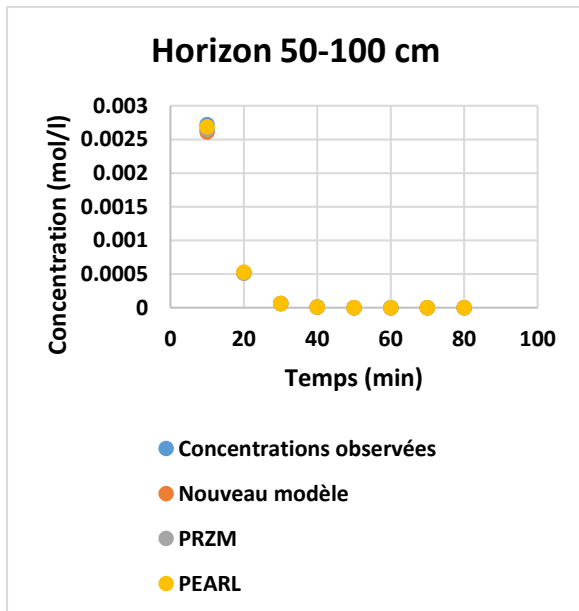


Figure 5: Comparison of simulation points between the new model and the PRZM and PEARL models on the 50-100 cm horizon

### C. DISCUSSION

The performance of the model was evaluated by calculating its efficiency using the Marin-Benito formula which compares the values simulated by the model to the real values obtained experimentally. This performance was evaluated at 0.97 for paraquat monitoring and 0.95 for glyphosate monitoring. These values being very close to 1, we arrive at the conclusion that the model simulates the evolution of pesticides in the soil very well, however, the performance of the model in simulating the transfer of paraquat being greater than that of the transfer of glyphosate, we conclude that the model simulates the transfer dynamics of paraquat than that of glyphosate.

Secondly, the performance of the developed model was compared to those of two existing models, namely PRZM and PEARL, for the transfer of mesotrione which is a herbicide over the horizons 0-20, 20-50 and 50-100 cm. It appears that the performance of the developed model was respectively 0.95; 0.94 and 0.93 for the three horizons, the performance of the PRZM model was 0.96, respectively; 0.97 and 0.94 for the three horizons and finally the performance of the PEARL model was respectively 0.98; 0.98 and 0.97 for the three horizons. It appears that the average performance values of these three models are close to 1, which means that these three models simulate the evolution of mesotrione in the soil well. However, the performance of the PEARL model was above the performance of the other two, followed by the PRZM model and finally the new model, which means that the PEARL model best simulates the evolution of mesotrione followed by the PRZM model and finally the new model developed. To better understand these comparisons, the MAPE(%) and RMSE values were calculated for each model. The MAPE (%) values for the new model were -2.17, respectively; -1.66 and -3.88 for the three horizons, those of the PRZM model were respectively -0.69; -0.49 and -2.81 for the three horizons and finally those of the PEARL model were respectively -0.33; -0.28 and -2.68 for the three horizons. The first observation is that all these values are negative, which means that the three models underestimate the real values obtained in the field. On each horizon, the MAPE values are the smallest in absolute value among the three, followed by the PRZM and PEARL model, which confirms the fact that the PEARL model is the best of the three, followed by PRZM and the new model.



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