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IMPROVEMENT OF THE INTERACTIONS BETWEEN THE UNSATURATED AND THE SATURATED ZONES: IMPACT ON POLLUTANT TRANSFER

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1 INTRODUCTION

A side effect of the intensive use of fertilizers in the agricultural activity since the 50's is a diffuse nitrate contamination in the aquifers. In the Seine basin, the nitrate concentrations in the aquifers are rather high and the drinkable water supply of the Paris urban area can be at risk. In order to estimate the evolution in time and space of a contamination in this hydrosystem and test the impact of remediation policies, a coupling between an agronomical model Stics and a hydrogeological model Modcou was implemented[2].

This model is able to represent the temporal evolution of the average nitrate concentration for the three main aquifers of the Seine basin, but some large local errors occur. In order to improve this modelling, special attention is given to the simple scheme of the unsaturated zone (UZ) in the MODCOU model. Indeed, this medium is responsible for the delay for nitrate to reach the water table. This delay can be rather long since the transfer through the UZ varies from 0.5 m/year to 2 meters/year[1]. We have therefore improved the modelling of the solute transfer in the UZ based on results of comparison with a physically-based model.

This paper presents the new UZ transfer scheme and its assessment. Then the new model is applied on the Seine basin, and the impacts on the groundwater contamination are presented.

2 IMPROVEMENT OF THE LARGE SCALE UNSATURATED ZONE MODEL NONSAT

Nonsat is a conceptual model simulating the 1D vertical transfer of water and solute through the UZ using a Nash cascade[3]. Nonsat assimilates the UZ to a series of *N* reservoirs *i* of a given thickness *d*, flowing in each other. Each reservoir follows an exponential law.

In order to take into account the immobile phase that contributes to solute storage in the UZ, a minimal volume *Vmin* has been introduced in Nonsat². *Vmin* is set identical in all the reservoirs of an UZ column.

When an infiltration occurs at a time step, a stratum is introduced at the top of Nonsat. Strata, defined by a given water volume and a given concentration depending on pedo-climatic and agricultural conditions at the current time step, pile up in the reservoirs². This stratification limits any mixing within the whole reservoir.

Then a piston effect occurs: an inflow at the top of the reservoir leads instantaneously to an outflow at the bottom of the reservoir. If the outflow includes several strata, they are mixed.

For numerical reasons, a maximum number of strata is set. When this maximum is reached, a mixing occurs: two strata near the *Vmin* are mixed together.

These mixings lead to diffusion. However, this diffusion is still limited.

The continuity of flow between reservoirs i and i+1 is therefore written:

$$Vin_{i+1(t)} = Vout_{i(t)} = \left(Vol_{i(t)} - V_{\min(i)}\right)\times\delta \tag{1}$$

with $Vin_{i+1(t)}$ the inflow into reservoir *i+1* (m^3), $Vout_{i(t)}$ the outflow of water from the reservoir i (m^3), Vol_i the volume of water in the reservoir *i* (m^3), δ a drainage coefficient, *i* the reservoirs index ranging from *1* to *N*, $Vmin_i$ the minimal water volume in the reservoir *i* (m^3) and *t* the current time. δ is linked to a percolation time τ in days by the relationship $\delta = 1 - e^{\frac{dt}{\tau}}$ with *dt* the computation time step (one day).

Nonsat has therefore 4 parameters: τ, that is set according to the soil type; *N*, that is set depending on the average thickness of the UZ and the given depth of the reservoir *d*; the maximal number of strata that is set uniform in the whole domain; and *Vmin* that can vary in space according to the soil type. As initial conditions, the water volume in each reservoir of an UZ is equal to the defined *Vmin*.

In order to improve this simple scheme, two main modifications are introduced: a varying saturation profile and a varying percolation rate. This new version is referred to as NonsatVG.

2.1. Introduction of a varying percolation rate

τ is related to the time in days required to entirely drain a reservoir. A percolation velocity can therefore be approximated from this data. As τ is constant in the UZ column, the percolation velocity is considered to be constant. However, the velocity should vary according to the saturation.

In order to take this process into consideration, we use a generalisation of Darcy' s law for the saturated zone by assuming that the water transfer is proportional to the saturation. The $Vin_{i+1(t)}$ (or the $Vout_{i(t)}$) is therefore multiplied by a coefficient of percolation *coef*:

$$coef = \frac{Vol_{i(t)}}{por \times S \times d} \tag{2}$$

With *por* the porosity ($m.m^{-1}$) and *S* the surface of the grid cell (m^2). Indeed, when the saturation fraction increases in the reservoir, the outflow increases to.

2.2. Introduction of a saturation profile

The UZ is subject to an evolution of the water content through the column, from its base that is almost saturated, to its top that is drier when the equilibrium is reached. The water retention curve in a UZ can be described by the Van Genuchten’s equation[4].

Figure 1 presents the evolution of the saturation profile as a function of depth in a loamy soil as described by Van Genuchten (Metis) for a given set of parameters. In Nonsat, the saturation profile at equilibrium for this type of soil is constant in each reservoir and equal to *Vmin* through all the reservoirs of the UZ (dotted line in Figure 1).

To improve the realism of the model, a saturation profile is integrated in Nonsat based on the Van Genuchten' s retention curve.

This leads to a variation of the minimum volume *Vmin* between each reservoir as presented in Figure 1 for a loamy soil (NonsatVG).

For each reservoir, *Vmin* is computed as follows in NonsatVG:

$$V_{\min(i)} = \int_{bottom_i}^{top_i} \frac{1}{\left[1+\left(\alpha\times\phi_x\right)^n\right]^m} \times por \times S \times \Delta z \tag{3}$$

With α, n and m the curve parameters, z the depth and φ the capillary pressure head (m) that depends on the water table depth. This leads to a variation of the *Vmin* between each reservoir. As the water volume of the reservoirs increases with the depth, the time transfer of the solute increases too, whereas the velocity transfer is constant in the former version of Nonsat.

2.3. Fluctuations of the water table

The introduction of the Van Genuchten’s profile in Nonsat allows integrating a direct link between the UZ saturation and the water table depth. The effects of the water table fluctuations on the UZ can therefore be taken into account explicitly in Nonsat. The problem is therefore the exchange of fluxes between the UZ and the aquifer. To deal with these exchanges, we make the following hypotheses: the hydrostatic equilibrium is reached instantaneously in the UZ and the water fluxes required for the equilibrium come from the saturated zone.

However, a small amount of water transferred from the UZ to the aquifer can lead to an important increase of the water table depth due to the differences between the definition of the porosity in the UZ and in the saturated zone. This latest is defined by an effective porosity and is thus usually smaller (30-40% for the total porosity in the UZ and less than 10% for the effective porosity in the saturated zone). Some preliminary tests are realised in an ideal case.

2.4. Parameters setting

One major difficulty with NonsatVG is that three new parameters are introduced, making it more complicated to calibrate on large scale domain. However, since the Van Genuchten's equation is widely used, some databases exist and can be used to provide these parameters. We therefore use the Carsel and Parrish[5] database as well as the parameters from Brouyère et al.[6] for chalk soil types.

3 ASSESSMENT OF THE NEW UNSATURATED ZONE SCHEME

An assessment of this new version is realized by comparison with a physically-based model Metis[7] and with in-situ data.

Metis is a finite element code solving the water and solute transfer equations in the unsaturated and saturated zones. It uses Van Genuchten's relationships[7] to describe hydrodynamic properties of UZ.

3.1 Assessment of NonsatVG in ideal cases studies

The dynamics of solute transfer simulated by Metis, Nonsat and NonsatVG are compared over a silty UZ column of 20m depth. As the schemes use different kinds of parameters and that, in those ideal cases, we are only interested by a comparison of the transfer dynamics in the UZ, we simulate a UZ depth from the Seine basin where the parameters for Nonsat were calibrated[2]. Metis is calibrated in order to obtain the same solute time transfer at the outflow of the column than in Nonsat. The first step is to have a similar water volume in the soil column of Nonsat by calibrating the porosity in Metis. Then permeability at saturation K_s is calibrated to fit Nonsat percolation velocity. Then the derived Van Genuchten's parameters and the porosity in Metis are set identical in NonsatVG.

These ideal cases are made with a constant infiltration (1mm per day) and an initial input of solute the first three days.

By construction, Nonsat is characterized by a solute transfer velocity constant through the time with no dispersion with depth. On the contrary, in Metis, the solute transfer velocity decreases with the depth and the solute dispersion increases in the deepest part of the UZ, due to the larger volume of water. The comparison has shown that this dynamics is well restituted by NonsatVG.

Moreover, whatever is the water table depth in Nonsat, solute velocity is constant. But in the Van Genuchten's equation, the water profile varies according to the water table depth. Thus in Metis and NonsatVG, the time needed by the solute to reach a given depth varies according to the piezometric level. This is illustrated in Figure 2. It shows the time needed by a passive solute to progress in a UZ for a water table located at 10, 15 or 20 meters depth. Due to the Van Genuchten profile in Metis and NonsatVG, the time needed by the solute to go beyond the first 5 meters is longer for a shallower UZ as the solute needs to flow through a greater volume of water and the percolation velocity decreases. Thus, the dynamics of the transfer is more realistic in the new version of our conceptual unsaturated zone transfer scheme.

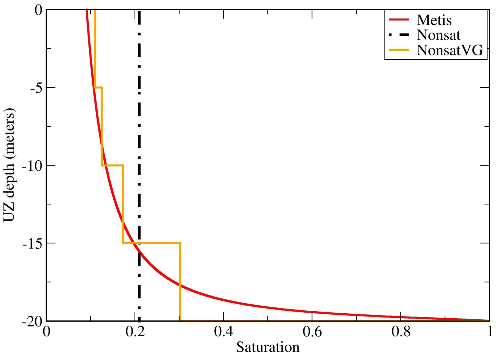

Figure 1: Evolution of the saturation with depth in Metis, Nonsat and NonsatVG.

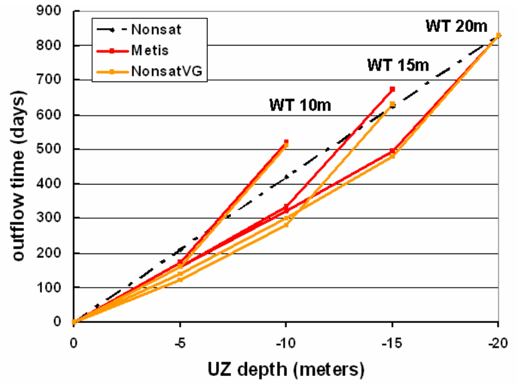

Figure 2: Time in days required for a passive solute to reach 5, 10, 15 and 20 meters depths in a loam UZ for three different water table depths (WT in meters) in Nonsat, NonsatVG and Metis.

3.2 Assessment of NonsatVG with observed data

The Agro-Impact group from INRA (National Institute in Agronomical Research) monitors nitrate concentration profiles at several sites. Figure 3 presents the observation in the chalky UZ of Haussimont (48° 45’ 0’’ North – 4° 10’ 0’’East), in the Seine basin. These profiles located 1 to 20 meters deep are available from 1982 to 2004. The propagation of a nitrate peak over time can be observed. These observations were used to assess the UZ scheme.

To do so, the nitrate concentration profile of 1982 is imposed as initial condition and no more additional nitrate input is supposed. The water percolation flux is determined with the water balance module of MODCOU[1]. Daily precipitation and potential evaporation data are provided by the SAFRAN analysis of MétéoFrance[8]. A constant depth of the water table is assumed and is set equal to 25 meters depth according to neighboring piezometric wells.

Parameters defined by Gomez[6] over the Seine basin for chalky UZ are used in Nonsat. For Metis and NonsatVG, we use parameters defined by Brouyère[6]. The dispersivity in Metis is set at 12.5cm, according to the simulation of the LIXIM model[9] used by INRA.

Metis simulates an evolution of the concentration profile that is close to the observed one (average transfer velocities (AVT) are respectively 0.4m/year and 0.5m/year). The depth of the peak for each given date and the diffusion are however slightly underestimated comparing to observed data. Solute peak is transferred too quickly in Nonsat (2.5m/year). Profiles simulated by NonsatVG are improved comparing to Nonsat. The AVT is however too slow (0,44m/year) and the dispersion does not compare well to the observed one.

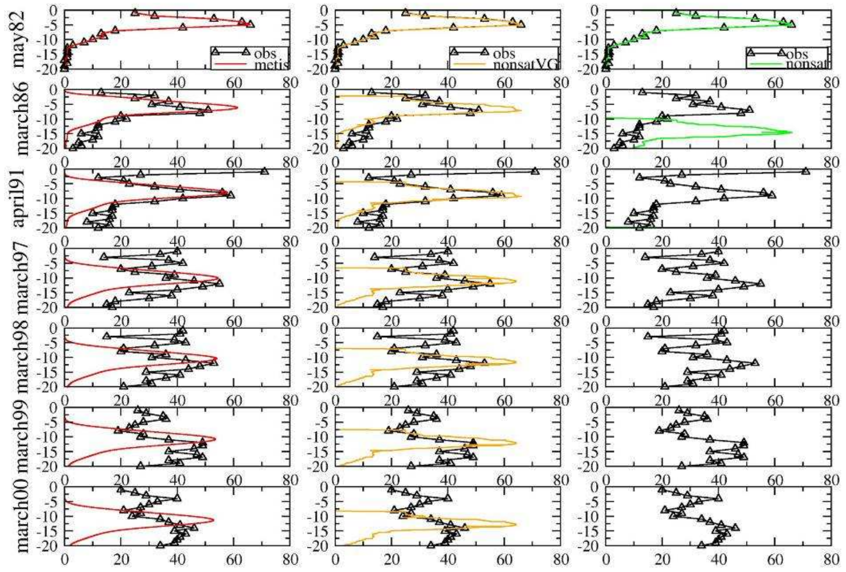

Figure 3: NO_3 concentration profile in mg/L (x axis) at Haussimont from 1982 to 2000 in a UZ of 25 meters depth (y axis) and simulated by Metis (red curve), NonsatVG (orange curve) and Nonsat (green curve).

Nonetheless, the simple UZ scheme NonsatVG obtains reasonable results and a large improvement compared to the original version. Comparable results are obtained in another experimental site, Thibie[10].

4 APPLICATION TO THE SEINE BASIN

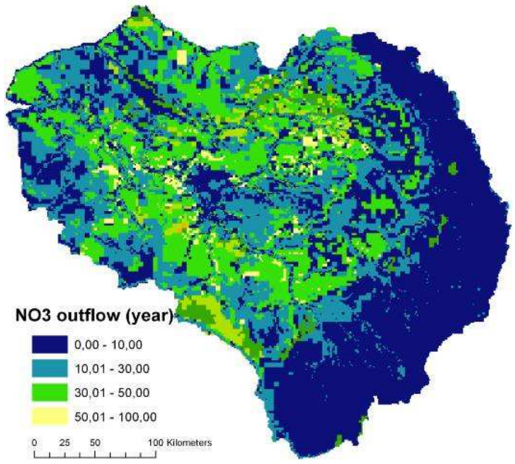

Figure 4: Averaged time required in years for a nitrate transfer through the UZ in the Seine basin with NonsatVG.

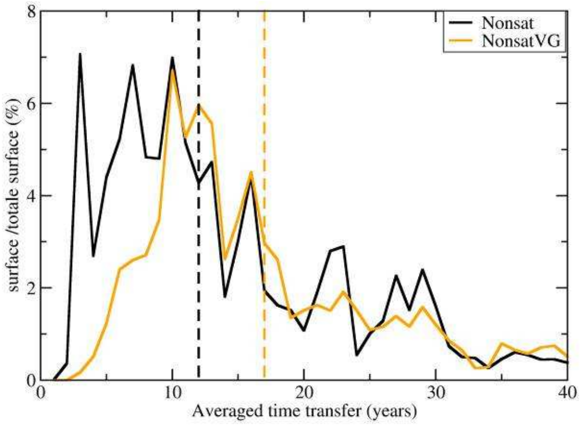

Figure 5: Surface repartition of the Seine basin depending on the averaged time required in years for an outflow of nitrate from the UZ to the saturated zone. At the dashed line, 50% of the UZ in the basin have transferred nitrates to the saturated zone.

It was shown that the new UZ scheme obtained quite different results from the former one. In order to quantify the impact of such differences in the pollutant transfer of the Seine basin, we first compare the UZ time transfer dynamics in this area.

A 35-years simulation was done supposing an input of passive pollutant at the beginning of the simulation and the real atmospheric forcing imposed from 1971 to 2006. The infiltration in the UZ is computed by MODCOU[3]. Figure 4 presents the map of the solute time transfer through the UZ in the Seine basin obtained with NonsatVG. More than 50 years are easily required for the solute to reach the groundwater where the aquifer is deep. This transfer is longer than with Nonsat. Indeed, with the former version, 12 years are required for a solute to reach the water table in 50% of the basin, while it is 17 years with NonsatVG (Figure 5).

Then, a first attempt was made to try to reproduce the observed nitrate concentration in the 3-layers aquifers of the Seine basin. To do so, we use the agro-hydrological model Stics-MODCOU[2] and NonsatVG instead of the former UZ scheme. We use the agronomic database[11] available from 1970 to 2005, and the atmospheric forcing from SAFRAN.

One problem is linked to the initialization of the concentration in the UZ and in the aquifer prior to 1970. As a first attempt, we use the same method as in Ledoux[2], ie, simply a spin-up by repeating a forcing during 35-year. Figure 6 presents the comparison between the observed and simulated mean concentration on the 3 aquifers of the Seine basin, for both the original and new version of the UZ schemes. NonsatVG has a smoother evolution of the mean nitrate concentration in each aquifer of the Seine basin than Nonsat, which was expected since the time transfer is longer in average, thus the mean window is larger.

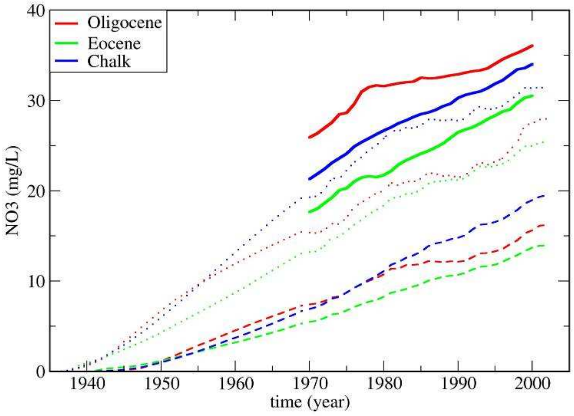

Figure 6: Evolution in the three main aquifers of the Seine basin of the observed nitrate concentration median and the mean nitrate concentration simulated by Nonsat (dotted line) and NonsatVG (dashed line).

However, it is not possible to have a more detailed comparison with the observations, since it can be seen that the nitrate concentrations at the beginning of the simulation are not in good agreement with the value of the median computed from observed data (especially for the Oligocene). These discrepancies are probably due to the initialization method that is too simple and not consistent with the few long-term available data. Indeed we suppose that no nitrate is present in the aquifer in 1935, while the long term observations show nitrate concentration around 20mg/L in 30's. Moreover, our initialization method supposes a constant input of solute occurs during 35 years while it is known that there is increasing use of fertilizers since the 30's. A better initialization method based on a better estimation of nitrate concentration in groundwater from 1930 is therefore under way.

5 CONCLUSION

We developed an improved version of a simple UZ scheme dedicated to large scale, and presented some comparison with a physically based model in ideal and real cases. This UZ scheme is used in the STICS-MODCOU chain[2], and leads to a new estimation of the nitrate concentration in the three main aquifers of the Seine basin However, the results are difficult to analyze while a better initialization method based on available information is not build.

The next step is thus dedicated to have a realistic simulation of the nitrate concentration of the aquifer of the Seine basin over a longer period. Then the impact of the fluctuating water table depth will be studied.

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