COUPLED MODELLING OF WATER CYCLE AND NITRATE TRANSPORT IN A HYDROLOGICAL SYSTEM

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ABSTRACT

Nitrogen input due to agriculture is the major cause of groundwater pollution by nitrates. Nitrogen cycle which is responsible of the transfer of pollutant from the soil to the aquifers is governed by multiple and complex phenomena which have to be simplified before attempting its modelling. This paper proposes a nitrate leaching conceptual model into the soil taking into account nitrogen input and agricultural techniques effects. This model is compatible with a spatially discretized representation of both surface and ground flow model already developed by the authors. This model has been validated to a lysimetrical case scale as well as to the scale of a small french cultivated watershed.

Results are meaningful and allow future utilization in studies for prevision of the ground water quality related to agriculture.

INTRODUCTION

Nitrogen, particularly under its nitric species (NO_3-) is one of the principal elements used in the nutrition of beeings. However, this need is limited and nitrogen may become a pollutant when its quantity overcomes a certain amount. In potable water for man, for instance, this amount is limited to 50 mg/l of nitrates in C.E.E. countries as defined wy WHO.

At the scale of the earth, the main input of nitrogen in ground comes from natural fixation from the one contained in the air; however, it is the production of fertilizers which predominates in populated areas. Nowadays, it seems clear that the major nitrogen pollution in the water is caused by the intensive agricultural activities.

Even though the situation has become alarming, there is no evidence of a solution in the near future. Due to the fact that the nitrates before becoming pollutants are nutrients, a balance between the soil productivity and the quality of the environment is not easy to measure and to preserve.

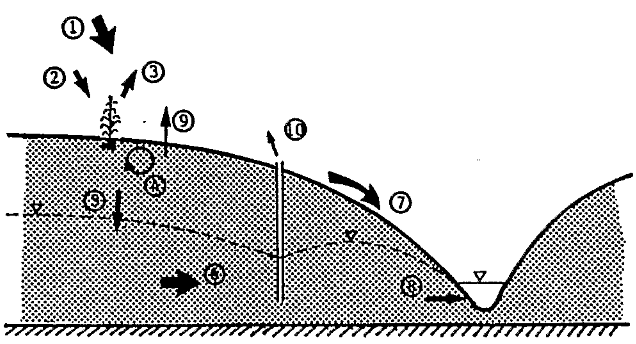
This problem is therefore the one of an optimization in the use of nitrates in the soil-water-plant system where a lot of important natural and human factors are included which can be resumed by a competition between the nutrient intake by the plants and the one dragging by water. Modelling may contribute to that objectif.Our objectif is to present a model that could, first, simulate the behaviour of an hydrogeological and agricultural system and, secondly, provide the system managements with the information on the future of the potential pollution of that system under different scenarios of human activities. It is rather difficult for the manager to obtain precise and sufficient information whenever they want to use empirical models. That is why one should use the phenomenological models where the variables and parameters have physical meaning and are measurable.

But to this scale, certain more rigorous phenomenological approaches are not applicable in practice, either because of lack of data, or because of a large set of parameters to be introduced in the use of the model. This leads to a compromise of suiting the phenomenological and parametric approaches according to the need and a pragmatic oncoming.

1. GENERAL ORGANIZATION IN THE MODELLING OF NITRATES TRANSFER

The modelling considers the representation of different phenomena (see fig.1):

- hydric balance and water runoff;
- nitrogen cycle and balance as well as leachate of nitrates into the soil;
- nitrates migration in the aquifer system.



1. precipitation; 2. N input (fertilizer);
3. input-output by crops; 4. internal transformations; 5. leaching; 6. groundwater transport; 7. surface water transport;
8. surface water-groundwater exchange;
9. return to the air; 10. pumping discharge.

Figure 1. Nitrates transfer scheme in a hydrological and agricultural system at a regional scale

The modelling of the water flow and the migration of a soluble conservative substance in an aquifer has been performed in several studies. We have begun our study from the spatially discretized hydrological models already developed and known as "the coupled model" MC (Ledoux, 1980) and NEWSAM(Marsily et al., 1976) model. We then developed a model representing the nitrogen balance and nitrates leachate called MORELN which uses the same spatial discretization as the before mentioned models and is totally compatible with them.

The basic idea is to provide the MC model with a function simulating the transport of a pollutant of agriculture origin, like nitrates.

In a complete hydrological system like the one represented by the MC model, one can distinguish, according to time and space residence of a pollutant, four different categories in the transport:

- transport in the soil, essentially the nitrogen mass balance determined by agricultural applications, water balance and the climatic factors;
- transport in the unsaturated zone, which traduces the lag-time in leaving the soil and entering the aquifer;
- transport in the aquifer system, governing the spatial distribution and the evolution of pollutant concentration in time;
- transport in the surface, more particularly in the drainage system interacting with the groundwater aquifer.

The key point is the first type of transport where the nitrates production is regulated defining the input function of the pollutant into the system. The elaboration and validation of the model representing this function constitutes the essential part of the research.

2. THE NITROGEN CYCLE IN THE SOIL

The nitrogen cycle in the soil is a complex phenomena which includes the interaction of several processes which we classified in three categories (see fig.2).

- Processes governing the nitrogen input:
  - biological fixing of atmospheric nitrogen by plants;
  - input of mineral nitrogen by precipitations;
  - artificial contributions (agricultural practices, spoils);

- Processes governing the nitrogen output:
  - bacterial denitrification;
  - volatilization of gaseous nitrogen;
  - leaching of nitrates by infiltration.

Processes governing internal transformation:

- ammonification from organic nitrogen to mineral nitrogen by bacteria;
- nitrification from ammoniacal nitrogen to nitric nitrogen by bacteria;
- reorganization, assimilation by micro-organisms;
- adsorption-desorption of ammoniac by the soil.

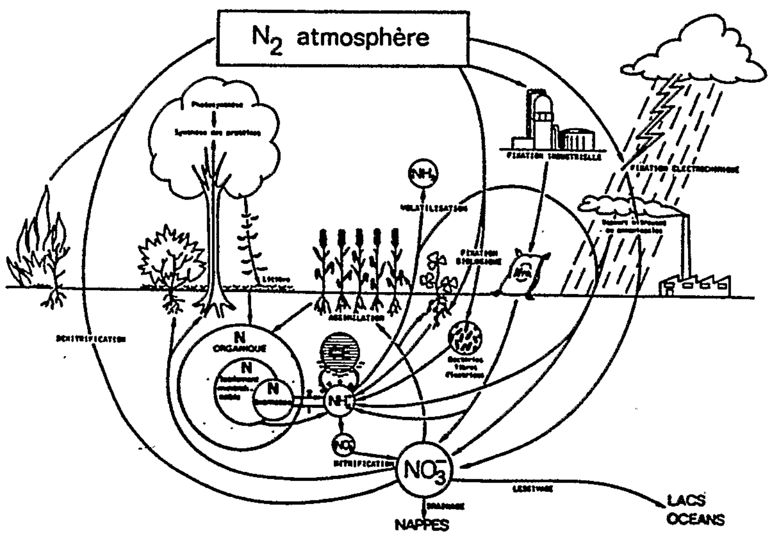


Figure 2. General representation of nitrogen cycle (from Mariotti, 1982)

3. MODELLING OF THE NITROGEN CYCLE IN THE SOIL

The nitrogen cycle in the soil is extremely complex. Because of the lack of knowledge of certain phenomena and the lack of data to be used in a very detailed modelization, we will adopt some simplifying assumptions in order to make possible the modelling exercices.

Generally, there exists no data on the composition of organic nitrogen in the soil. So we will consider it as homogeneous and under a unique forme where the mean composition will reflect the mineralizable part at the time scale considered by the simulation.

The state of the knowledge and data availability does not allow us to take into account the soil-atmosphere interchange phenomena in the modelling. For this reason, we will suppose that the input (precipitation + biological fixing) and the output (denitrification + volatilization) terms globally compensate;

Because of the rapidity in the nitritation according to the nitratation, we will consider that nitrification is done in a single stage governed by the slowest speed (nitratation). In other words, we will neglect the (NO_3-) species in the representation of the nitrogen cycle.

Finally, we assume that the processes of the uptake by plants and leaching by water only concerns the nitrates.

The simplified nitrogen cycle may be represented as follows:

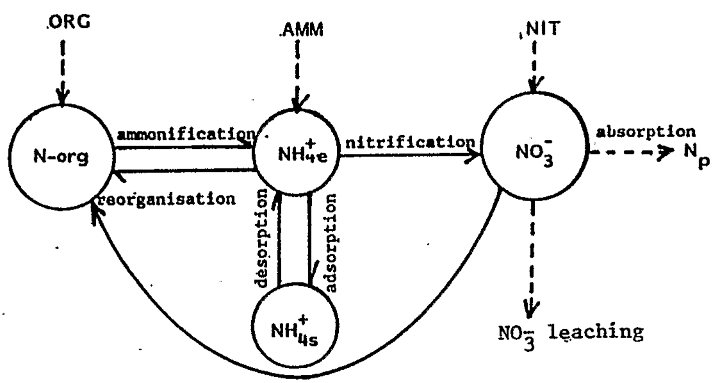


Figure 3. Diagram of the simplified nitrogen cycle for the modelling

Each part of the process described above is represented mathematically, and implemented in the model in space and time, allowing the estimation of a nitrates leaching term which is then introduced into the ground transport model (Geng, 1988).

There are two categories of data introduced in the MORELN model:

- . the data from the hydrological model MC, including precipitation, runoff, infiltration and moisture storage;
- . the agricultural and pedological type of data due to the model MORELN. These are the contributions from fertilizers, irrigation practices, thickness, density and water capacity of the superficial soil.

The parameters are divided into three categories:

- the nitrogen potential consumption used by the field crops and the absorption coefficient. The former can be evaluated from the field and the latter can be determined by calibration of the model;

- the kinetic coefficients of the four internal biochemical transformations. They play the indirect role in the calcul of the leaching flux and the uptake of nitrates. Their estimation by calibration of the model is less rigorous due to the fact that these four processes are not precisely known in general;

- the correction coefficients of the preceeding coefficients as function of the soil temperature. In this case, reported values will be taken.

The results in the output of the model are principally the leaching flux of nitrates and the consumption in nitric nitrogen by the crops. These are the two most important results which characterize the behaviour of the soil-water-plant system and the easiest to check. Additionally, the model also estimates the reserve of nitrogen substances of the different compartments and the flow of the four internal biochemical transformations, which will eventually be confronted with the the observations in the field.

4. MODEL VALIDATION ON A LYSIMETER

A first validation of the nitrates leaching model was performed using the data of an experiment in a lysimeter by the National Institute of Agronomic Research (INRA) in Versailles (France).

The box used is a parallelepiped of 2 m² in the surface and over 1.5 m depth. The fill material is homogeneous over the depth and is constituted mainly by silty soils.

The box has a free drainage open device and the water is capted at the bottom. Measurement of the drained water was done daily, while the chemical analysis of water was done rather irregularly, varying from some days to two weeks.

The crop rotation in this box is wheat-corn. The occupation period of wheat goes from November to August between the dates of sowing and harvest. For corn, this period goes from end of April to October.

The box receives the fertilizers essentially in spring, representing a nitrogen input equivalent to a 130 and 160 kg N/ha dose by crop cycle. There is an additional and frequent input of nitrogen in autumn by reincorporating the residual after the harvest accompanied sometimes by a complementary input of ammoniacal nitrogen evaluated to some tenths of kg N/ha.

Results over 10 years of simulation are shown in Table I:

Year	73 - 73	74 - 74	75 - 75	76 - 76	77 - 77	78 - 78	79 - 79	80 - 80	81 - 81	82 - 82
Type of culture	C	W	C	W	C	W	C	W	C	W
Observed drainage (mm)	91	101	37	127	224	94	168	71	187	122
Computed drainage (mm)	86	103	31	126	222	101	115	62	180	107
Observed N leaching (kg N/ha)	7.0	8.4	3.1	28.	67.	2.8	15.	1.2	21.	5.7
Computed leaching (kg N/ha)	9.1	7.8	3.0	6.6	30.	3.7	11.2.3		20.5.6	

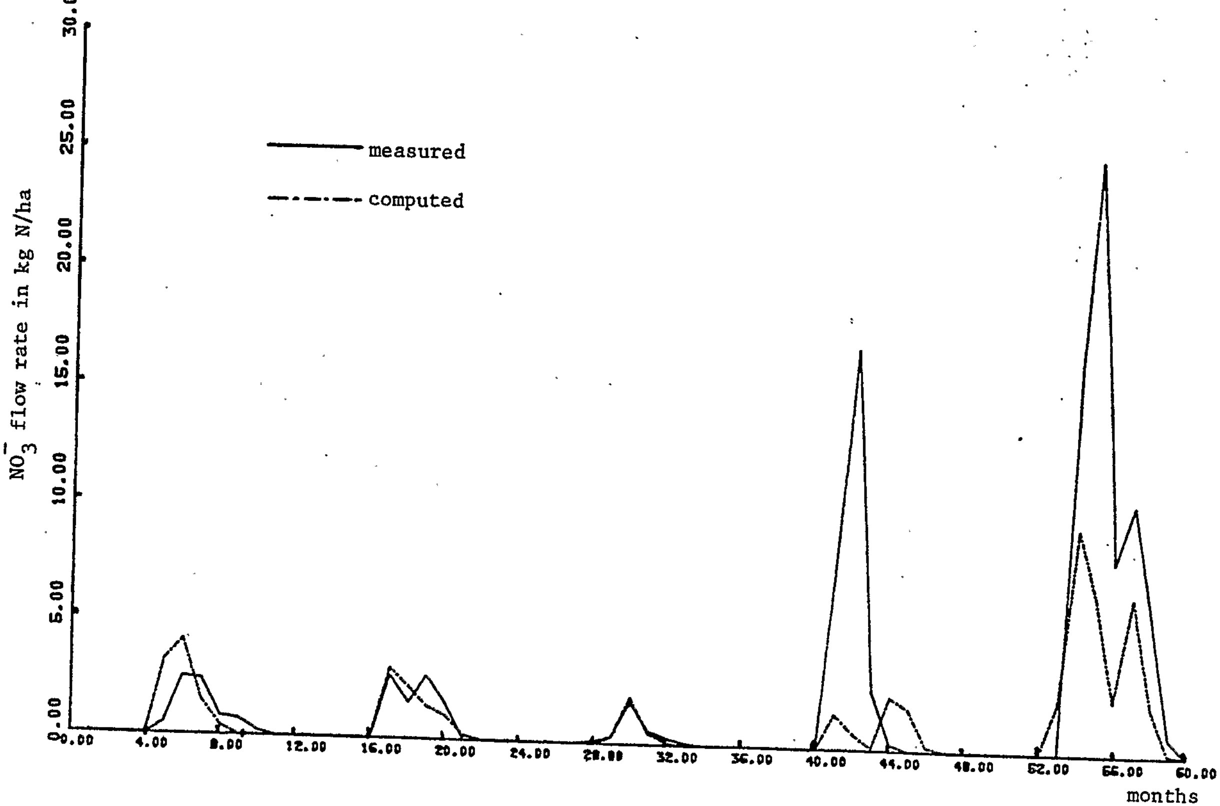
C = corn W = wheat

Table I. Comparison between annual observed and estimated leaching.

Due to the fact that leaching of NO_3- is strongly influenced by water drainage, the trend of the leaching curve follows very closely the one of the drainage.

In the two years (76-77 and 77-78) following a great drought period (75-76), the difference between the estimations and observations is important, estimated leaching is greatly inferior to observed leaching (fig.4). This can be explained by an accretion of mineralization of organic nitrogen as shown by some experiences in the laboratory (Mariotti, 1982), where the speed of the mineralization of samples pre-dried in the air is accelerated compared to normal samples. This phenomenon, known as "flush effect" is explained by the destruction of soil biomass (Mariotti, 1982). We think that

FIGURE 4. NITRATE LEACHING FROM A LYSIMETER



such a phenomènon has indeed happened in the lysimetric box following the great drought of 1976. This is not taken into account in the model, which considers that the kinetic of mineralization is unchangeable.

Agricultural data	Type of culture	Observed consumption	Estimated consumption
08/05/74-30/10/74	Corn	157.1	124.6
05/12/74-29/07/75	Wheat	158.6	163.8
23/04/76-16/09/76	Corn	107.3	158.9
26/10/76-16/08/77	Wheat	214.7	147.9
12/05/78-31/10/78	Corn	243.2	186.4
22/11/78-14/08/79	Wheat	129.7	133.6
29/04/80-20/10/80	Corn	209.2	157.4
29/10/80-12/08/81	Wheat	136.3	152.1
21/04/82-18/10/82	Corn	201.1	202.6
23/11/82-03/08/83	Wheat	138.8	155.7

Table II. Comparison between estimated and observed consumption.

Besides leaching, another important result in the model is the estimation of nitrogen consumption by the crops. Table II shows the comparison between observed and estimated consumption. We can see that estimated values are in general very close to the observed ones. Like for leaching, the model gives smaller values compared to the observations for the two years after the drought period.

We can say that in general the model has correctly simulated the water and the NO_3- flow through the soil as well as the nitrogen consumption by the crops. Values of parameters concerning the kinetics of nitrogen biochemical transformation in the soil are quite consistent with those cited in the literature. A conclusion in our approach is the proposal of the values for the parameters which characterize the nitrogen absorption by the roots which should be critisized in other applications.

Extreme climatic events may considerably disturb the nitrogen cycle in the soil. The great drought of the year 1976 has greatly amplified the mineralization and nitrification in the soil during the two following years. The model should be modified and adapted in order to take those disturbances into account in which the mechanisms are not yet fully quantified.

To a lysimetric box scale, the soil behaviour with respect to drainage and leaching is very sensitive to changes in soil occupation (crops rotation) and to tilling.

5. MODELLING NITRATES TRANSPORT IN A SMALL EXPERIMENTAL WATERSHED

The example chosen is the watershed of the Noë-Sèche, located in Bretagne, in the west of France. This basin, situated in a granitic region, has been studied in detail, investigating the agricultural activities and the nitrogen balance during the year of 1983.

The site is a small drainage basin in which the surface area is only of 576 ha. Even though there seems to be a groundwater aquifer relatively developed compared to other basins in the region, its importance is limited according to nitrates transport as compared to other processes of rapid transport manifesting during the floods. This hypothesis seems conforted by measurements of nitrates flux in the river in which high values coincide with high rates of flow. Besides, we do not dispose of any data to characterize that aquifer. So we will admit that the dominant phenomenon to the basin scale is production and not displacement; in such a way, we consider, in the modelling, the basin to be a great box lysimetric of polyculture.

AVAILABLE DATA

- Flow rates and nitrates content:

Data are available on a daily basis for the period March 1983-February 1984, flow rates are measured in a gauging station at the outlet of the Noë-Sèche basin.

Water chemical analyses give concentration in NO_3^-. This analysis is done every three days in average. In the simulation, the values of the preceding days will be given to those days without data.

With these two series of data, we will estimate a flow of NO_3^- that will be used in the calibration process.

- Meteorological data:

A rain gauge in the site has registered, for that period, a precipitation of 967 mm.

Decadal data of temperature in the soil and potential evapotranspiration (Penman) are available in a nearby meteorological station.

- Agricultural data: Nitrogen inputs into the basin

In the first place, we have a daily schedule of fertilizers application in the form of mineral and organic fertilizers in sites not spatially localized.

Because of the three types of chemical forms of nitrogen used in the model (N organic, N ammoniacal and N nitric), the inputs should be converted into those three forms.

In the second place, besides those inputs valorized to 100% for the crops, there also exists other quantities of nitrogen coming from different parts (dejections in the highways, different leakage of effluents, etc...). Those nitrogen quantities are considered as "direct losts" for the crops, but they should be considered as inputs in our modelled hydrogeological system, it is convenient to take them into account in the total balance.

Those quantities (N) have only been estimated annually. In order to distribute them in the time (on a daily basis), we have supposed that the contributed quantity is proportional to the number of grazed animals.

Finally, we have also taken into account the nitrogen contained in the crops roots, reincorporated into the soil under the form of organic N after the harvest.

- <u>Data concerning field crops practices</u>:
These data are used to estimate the potential consumption of nitrogen by the crops. They are available in the basin for the cereal crops.

Concerning the meadows, things become more difficult: we do not know the rythm and the intensity of the grazing, by the effect of mowing which perturbs the growing of meadows and so their nitrogen consumption.

Therefore, we have decided to use the results of a "grazing simulation".

<u>MODEL CALIBRATION AND ANALYSIS OF RESULTS</u>

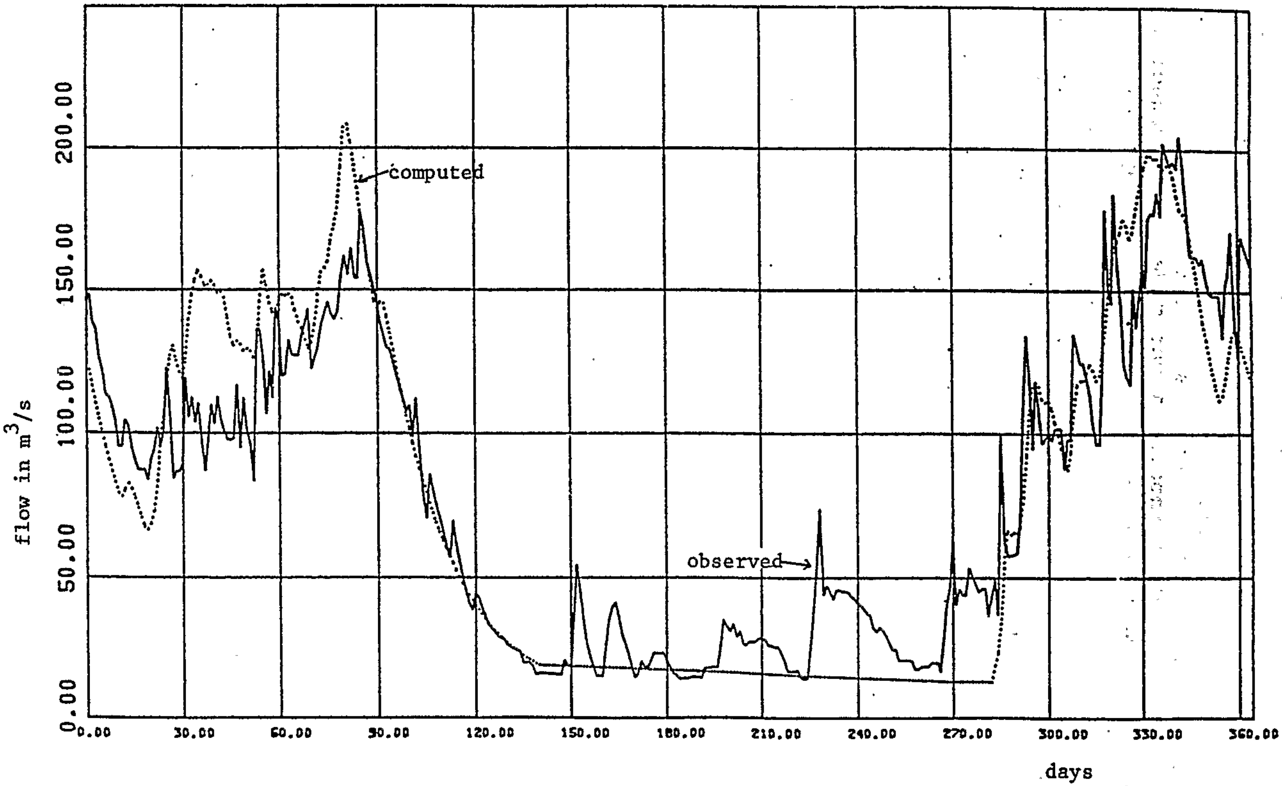
- A) <u>Calibration of the flow rate</u>:
Figure 5 shows the flow rate calibration results with a daily time-step. The model reproduces correctly, in the whole, the evolution of the measured flow rate except for two periods:

  . during the month of May, marked by an underestimation of the estimated flow rates;
  . at the starting of autumn, where the estimated flow rate curve rises more slowly than the observed one.

- B) <u>Calibration of NO_3^- transport</u>:
In this part of the calibration process, we will rather insist on the NO_3^- flow transported by the Noë-Sèche basin than on the concentrations for the following reasons:

. the evolution of the behaviour in the basin lies, we believe, on the regular seasonal variations of the NO_3^- flow rather than on the daily irregular fluctuations in concentration. The global model of the basin does not seem to have a good performance in simulating this last type of variability.

FIGURE 5. FLOW AT THE OUTLET OF THE WATERSHED



It is the impact of agricultural activities of the basin on the upstream area, e.g. the quantity (flow) of NO_3^- going out of the basin which is most worrying. Figure 6 shows the comparison between the observed and estimated NO_3^- flow on a daily time-step basis. It is clear, from the figure, that the leached NO_3^- flow curve is quite well reproduced, except for two periods:

- April-May, where the model estimates a higher NO_3^- flow as compared with the observed one. This may probably be a consequence, in the estimation, of the imprecision of the potential consumption of NO_3^- by plants during that period.
- As in the flow rate, the estimated NO_3^- flow curve rises more slowly than the one observed in the period starting in autumn. It then shows clearly the influence of hydrogeological factors affecting the evolution of pollution. Due to the fact that the concentration is rather constant, it is indeed essentially the flow rate which determines the flow of NO_3^-.

As a conclusion of the modelling exercices, we believe that:

1) The annual nitrogen balance over the basin is very lean:

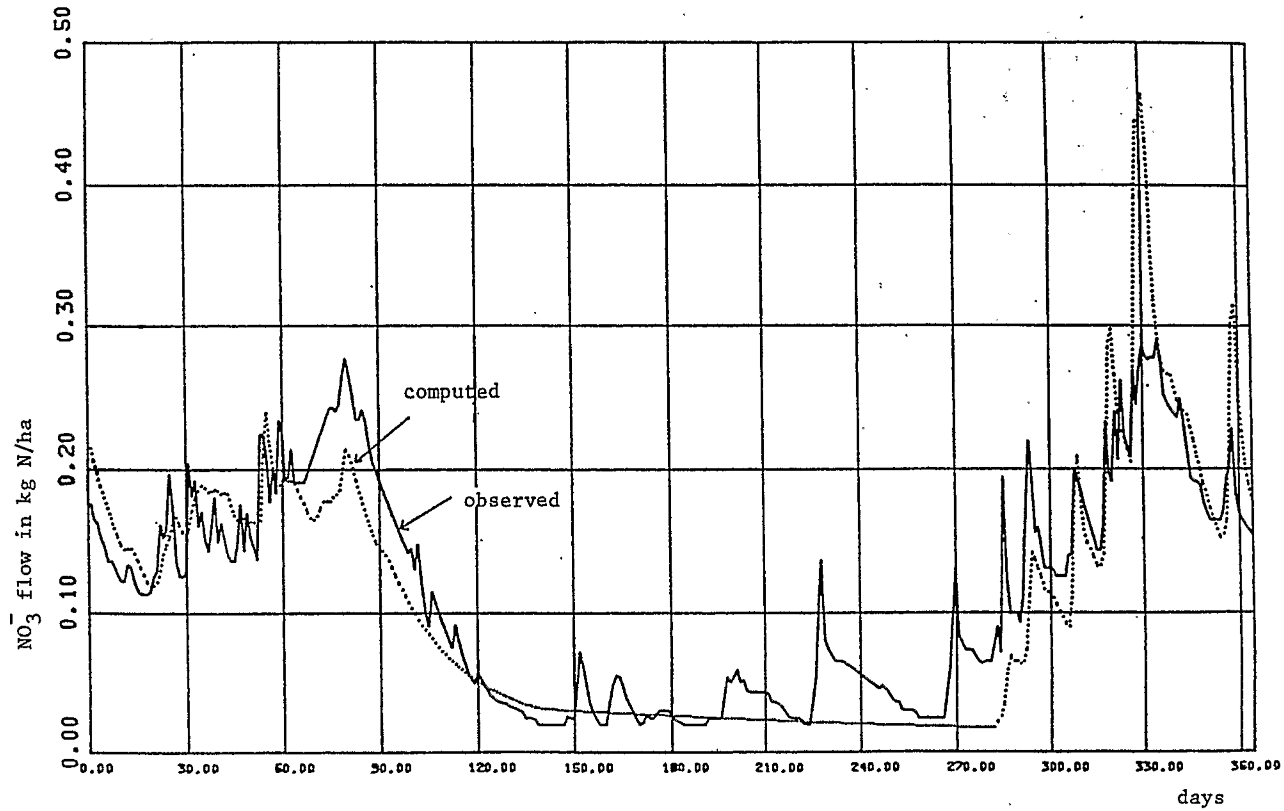
	Observed (kgN/ha)	Computed
Input in organic N	52	
Input in ammoniacal N	83	
Input in nitric N	43	
Total input	178	
Output from the Noë-Sèche	50	49
Output from crops	198	201
Total output	248	250
Total balance:	-70	-72

2) The NO_3^- exportation by the Noë-Sèche basin esti

mated in monthly and yearly terms agrees well with the measurements. The underestimation by the model for the months of October and November is quite understandable due to the fact that the flow rate, for the same period, has also been underestimated.

3) The NO_3^- consumption by the crops is well simulated. The simultaneous calibration of both the consumption by plants and the leached nitrates flow allows us to have a better control of the simulation of the whole nitrogen balance.

FIGURE 6. NITRATE LEACHING AT THE OUTLET OF THE WATERSHED



CONCLUSIONS

The proposed model for the transport of nitrates on a watershed lies essentially in a conceptualization of the nitrogen cycle in the soil, compatible with a spatially discretized hydrological model of a joint simulation of both surface and ground flow already developed by the authors.

The model has been validated to a parcell scale on the drainage and nitrates flow data obtained over several years on lysimeters. The extrapolation of the approach to a small drainage basin in polyculture has given good results showing a certain robustness of the nitrates leaching model concerning the parameter values considering the space scale in the study.

A foreseen utilization of such a model is the study of the influence of agricultural applications on the long range evolution of groundwater quality.

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