A hydro-economic modeling framework for optimal management of groundwater nitrate pollution from agriculture

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Abstract: A hydro-economic modeling framework is developed for determining optimal management of groundwater nitrate pollution from agriculture. A holistic optimization model determines the spatial and temporal fertilizer application rate that maximizes the net benefits in agriculture constrained by the quality requirements in groundwater at various control sites. Since emissions (nitrogen loading rates) are what can be controlled, but the concentrations are the policy targets, we need to relate both. Agronomic simulations are used to obtain the nitrate leached, while numerical groundwater flow and solute transport simulation models were used to develop unit source solutions that were assembled into a pollutant concentration response matrix. The integration of the response matrix in the constraints of the management model allows simulating by superposition the evolution of groundwater nitrate concentration over time at different points of interest throughout the aquifer resulting from multiple pollutant sources distributed over time and space. In this way, the modeling framework relates the fertilizer loads with the nitrate concentration at the control sites. The benefits in agriculture were determined through crop prices and crop production functions. This research aims to contribute to the ongoing policy process in the Europe Union (the Water Framework Directive) providing a tool for analyzing the opportunity cost of measures for reducing nitrogen loadings and assessing their effectiveness for maintaining groundwater nitrate concentration within the target levels. The management model was applied to a hypothetical groundwater system. Optimal solutions of fertilizer use to problems with different initial conditions, planning horizons, and recovery times were determined. The illustrative example shows the importance of the location of the pollution sources in relation to the control sites, and how both the selected planning horizon and the target recovery time can strongly influence the limitation of fertilizer use and the economic opportunity cost for meeting the environmental standards. There is clearly a trade-off between the time horizon to reach the standards (recovery time) and the economic losses from nitrogen use reductions.

Key words: *nitrogen management; diffuse groundwater pollution; hydro-economic modelling; optimization; Water Framework Directive*.

INTRODUCTION

Nitrate is among the most common and widespread pollutants in groundwater. Diffuse pollution from agricultural activities and livestock are often the main sources of elevated nitrate concentrations in groundwater (Nolan et al., 1997; EEA, 2003). Nitrogen is a vital nutrient to enhance plant growth, which has motivated intensive use of nitrogen-based fertilizers to boost up the crop production. But increased fertilizer use also has social and environmental costs. When the nitrogen fertilizer application exceeds plant demand and the denitrification capacity of the soil nitrogen can leach to groundwater, usually as nitrate, a highly mobile form with little sorption. Nitrate in drinking water has been linked to human health problems like methemoglobinemia in infants and stomach cancer in adults (Hatch et al., 2002; Wolfe and Patz, 2002), although the evidence for nitrates as a cause of these diseases remains controversial (Powlson et al., 2008). Excess nitrates in ecosystems can cause serious environmental damages, leading to eutrophication of connected surface water bodies that can eventually provoke algal blooms and fish kills. Agricultural non-point source pollution is the primary cause of water quality deterioration in many European watersheds (EEA, 1999 and 2003). Although the control of point source emissions improved the quality of many water bodies across Europe, nitrate concentrations in rivers from diffuse sources have remained relatively stable in Europe's rivers and groundwater, reflecting the large nitrogen surplus in agricultural soils and high livestock densities (EEA, 2003).

Water pollution has given rise to the development of an extensive legal framework. In Europe, the Nitrates Directive (Directive 91/676/EEC) was established in 1991 to reduce nitrate water pollution from agricultural sources, and involved the declaration of Nitrate Vulnerable Zones in which constraints are placed on inorganic fertilizer and organic slurry application rates. The Drinking Water Directive (80/778/EEC and its revision 98/83/EC) sets a maximum allowable concentration for nitrate of 50 mg/l. The EU Water Framework Directive (Directive 2000/60/EC; WFD), enacted in 2000, proclaims an integrated management framework for sustainable water use, and requires that all water bodies reach a good status by 2015. The good groundwater status implies both a good quantitative and a good chemical status. In addition to the groundwater status, any significant upward trend in the concentration of any pollutant should be identified and reversed (Directive 2006/118/EC, Groundwater Directive). The WFD explicitly recognizes the role of economics in reaching the environmental and ecological objectives. Different studies have been conducted to identify economically efficient groundwater pollution thresholds values (e.g. Brouwer et al., 2006).

Nitrate groundwater contamination results from several and complex processes from pollution sources to water bodies, including pollution formation (nitrogen leaching) and pollution reactions, fate and transport. Different methods have been reported to analyze the effects of policies on groundwater nitrate concentration and to find optimal levels of nitrogen use. Some studies focus on integrating of nitrate leaching into an economic framework to design nitrogen pollution abatement policies (e.g., Yadav, 1997; Martinez and Albiac, 2004 and 2006; Kim et al., 1996; Lee and Kim, 2002; Knapp and Schwabe, 2008). In these cases, nitrogen leaching is estimated using a wide range of soil-plant and nitrogen balance models, but nitrate transport and fate in groundwater is not considered. Therefore, the natural aquifer's ability to attenuate nitrate concentration is not taken into account. These approaches do not assess the resulting nitrate concentrations in groundwater, which are needed to assess if the standards are met or not. Other studies have applied a compartmental approach, in which the results of a nitrogen management model are tested using groundwater flow simulation models (e.g., Bernardo et al., 1993; Mapp et al., 1994). In this case, also the attenuation of nitrate concentrations within the aquifer is not considered.

A more detailed modelling of the bio-physico-chemical processes involved in nitrate transformation and fate and transport in groundwater is of great importance when designing optimal nitrogen abatement policies to control groundwater pollution in order to satisfy certain environmental constraints. Despite the considerable advances in the development of integrated tools for nitrate transport simulation at the catchment scale (ex. Refsgaard et al., 1999; Lasserre et al., 1999; Birkinshaw and Ewen, 2000) these modelling frameworks are not usually suitable for integration into management optimization models for identifying optimal policies. A few studies have proposed integrated economic-biophysical simulation approaches to assess the evolution of groundwater quality under different agriculture policies or protection measures, linking agricultural economic models with soil-plant, nitrogen balance, and groundwater flow and transport models (e.g., Gömann et al., 2005; Graveline and Rinaudo, 2007a; Graveline et al., 2007; Almasri and Kaluarachchi, 2007). In Almasri and Kaluarachchi (2005), a “black-box” statistical modelling approach (artificial neural networks) is used to relate on-ground nitrogen loadings with nitrate concentrations at specific control sites in a multicriteria decision framework.

The objective of this study is to develop a hydro-economic modelling framework for optimal management of groundwater nitrate pollution from agriculture. The optimization modelling framework explicitly integrates nitrate leaching and fate and transport in groundwater with the economic impacts of nitrogen fertilizer restrictions in agriculture. This research aims to contribute to the ongoing policy process in the Europe Union (the Water Framework Directive) by analyzing the cost of measures for reducing nitrogen loadings and their effectiveness on maintaining groundwater nitrate concentration within the target levels. With this method we contribute to the development of the programme of measures to be established by 2012.

NITRATE GROUNDWATER POLLUTION

Once nitrogen enters the soil, it undergoes several biochemical transformations before leaching to groundwater mostly as nitrate (Fig. 1). Losses in modern agriculture commonly account for 10-30% of the nitrogen additions (Meisinger et al., 2006). The transport and fate of nitrogen in the subsurface environment depends upon the form of entering nitrogen and the biochemical and bio-physico-chemical processes involved in transforming one form of nitrogen into others. Depending on the sources, nitrogen can enter the subsurface environment in organic or inorganic forms; nitrogen from chemical fertilizers will typically be in ammonium or nitrate form. The major sources of nitrates in groundwater include irrigated and rainfed agriculture and intensive animal operations (EEA, 1999). Septic tanks and other sources as landfills can leach nitrates in localized areas (Meisinger et al., 2006).

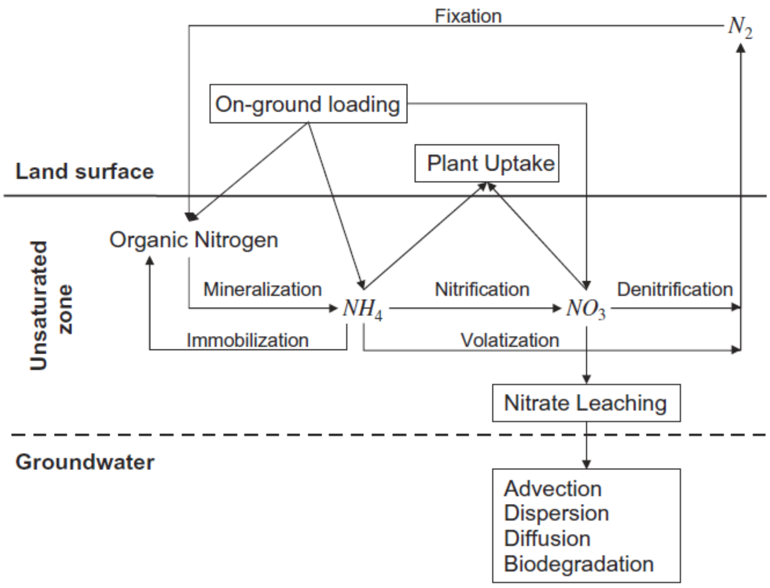

Fig. 1. Nitrogen groundwater pollution processes.

More than 90 % of the nitrogen in soil is organic, either in living plants and animals or in humus originating form decomposition of plant and animal residues (Canter, 1996). The nitrate content is generally low because it is taken up in synthesis, leached by water percolating through the soil, or subjected to denitrification activity below the aerobic top layer of the soil. However, synthesis and denitrification rarely remove all nitrates added to the soil from fertilizers and nitrified wastewater effluents (Tesoriero et al., 2000). Accordingly, nitrates leached from soils are a major groundwater quality problem. Accurate quantification of nitrate leaching to groundwater is difficult due to the complex interaction between land use practices, on-ground nitrogen loading, groundwater recharge, soil nitrogen dynamics and soil characteristics. Therefore it is important to understand the interaction of the aforementioned factors to account for the transient and spatially variable nitrate leaching to groundwater.

When nitrogen in the form of nitrate reaches groundwater, it becomes very mobile because of its solubility. Nitrates can move with groundwater with minimal transformation and can migrate long distances from input areas if there are highly permeable subsurface materials that contain dissolved oxygen. This process can be affected by a decline in the redox potential of groundwater that can lead to a denitrification process (Tesoriero et al., 2000). Groundwater fate and transport models are essential for assessing the impact of protection alternative measures that protect groundwater quality and reduce contamination.

METHOD

Management Model

An optimization model is developed to define efficient fertilizer allocation in agriculture: when, where and by how much fertilizer reductions have to be applied to meet the ambient standards (groundwater quality) in specific control sites in the aquifer.

The efficient allocation maximizes the present value of the net social benefit. The net social benefit equals the benefit received from the use of the resource minus external costs imposed on the society, including costs of damage from pollutants in the environment. Unless the level of pollution is very high indeed, the marginal damage caused by a unit of pollution increases with the amount emitted, and the marginal control cost increases with the amount controlled. Efficiency is achieved when the marginal cost of control is equal to the marginal damage caused by the pollution for each emitter. The optimal level of pollution is not necessarily the same for all locations. One way to achieve this equilibrium is to impose legal limits on the pollution allowed from each emitter, for the level of pollution where marginal control cost equals marginal damage. Another approach would be to internalize the marginal damage caused by each unit of emission by a tax or charge on each unit of emissions. To implement these policy instruments, we must know the level of pollution at which the two marginal cost curves cross for every emitter, which requires an unrealistically high information burden on control authorities (Tietenberg, 2002). Another approach is to select ambient standards, legal upper bounds on the concentration level of specified pollutants in water, based on some criterion such as adequate margins of safety for human or ecological health. The allocation of the necessary reduction of emissions for meeting the ambient standards can be achieved through cost-effective policies. A cost-effective policy results in the lowest cost allocation of control responsibility consistent with ensuring that the predetermined ambient standards are met at specified locations called “control sites”. Since emissions are what can be controlled, but the concentration at the receptor cites are the policy targets, it is necessary to relate both through the proper numerical simulation of the pollutants leaching, transport and fate within the aquifer.

In the proposed hydro-economic modelling framework, the non-point pollution abatement problem was stated as the maximization of welfare from crop production subject to constraints that control the environmental impacts of the decisions in the study region. Welfare was measured as the private net revenue, calculated through crop production functions and data on crops, nitrogen and water prices. The hydro-economic model integrates the environmental impact of fertilization by simulation of soil nitrogen dynamics and fate and transport of nitrate in groundwater with the economic impact (agricultural income losses) of water and fertilization restrictions, assessed through agronomic functions representing crop yields and crop prices. The decision variables of the problem are the sustainable quantities of nitrogen per hectare applied in the different crop areas (pollution sources) to meet the environmental constraints.

The management model for groundwater pollution control is formulated as:

$$Max\,\Pi = \sum_{c=1}^{n}\sum_{t=1}^{t}\frac{1}{(1+r)^{t}}A_c\left(p_c\cdot Y_{c,t} - p_n\cdot N_{c,t} - p_w\cdot W_{c,t}\right) \qquad (1)$$

subject to:

$$[RM]\{cr\}\leq\{q\} \qquad (2)$$

where Π is the objective function to be maximized and represents the present value of the net benefit from agricultural production (€) defined as crop revenues minus fertilizer and water variable costs (other costs are not included); A_c is the area cultivated for the crop c; p_c is the crop price (€/kg); $Y_{c,t}$ is the production yield of crop c at year t (kg/ha), that depends on the nitrogen fertilizer and irrigation water applied; p_n is the nitrogen price (€/kg); $N_{c,t}$ is the fertilizer applied to the crop c at year t (kg/ha), p_w is the price of water (€/m^3), and $W_{c,t}$ is the water applied to the crop c at year t (m^3); r is the annual discount rate, *[RM]* is the unitary pollutant concentration response matrix; *{q}* is a column vector of water quality standard imposed at the control sites over the simulation time (kg/m^3); *{cr}* is a vector of n elements which corresponds to the nitrate concentration recharge (kg/m^3) reaching groundwater from each crop area, whose components are given by:

$$cr_t = \frac{L_{c,t}}{r_t} \quad (3)$$

where r_t is the water that recharges the aquifer (m^3/ha) at time t, and $L_{c,t}$ is the nitrogen leached from each crop area (kg/ha) at time t. The sub-index t in the formulation refers to the year within the planning horizon or the number of successive years in which the fertilizer is applied.

The application of the optimization management model requires the integration of the soil nitrogen dynamics simulation (to define nitrate leaching) with the simulation of groundwater flow and nitrate fate and transport, so that on-ground nitrogen loadings can be translated into groundwater nitrate concentrations (Fig 2). Groundwater flow and transport governing equations are represented within the management model through the pollutant concentration response matrix *[RM]*.

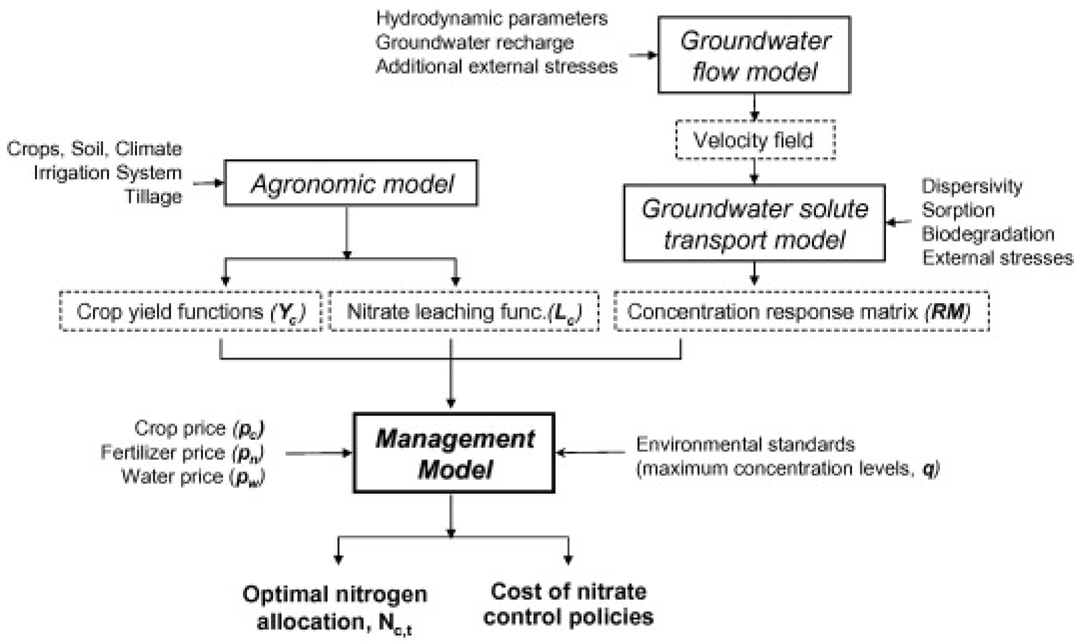

Fig. 2. Schematic describing the modelling framework

The method of embedding a numerical groundwater simulation model in an optimization management model as a series of constraints was first described by Aguado and Remson (1972). The number of model constraints defined using classic numerical methods can be excessively high, especially in hardly discretized aquifers (Peralta et al., 1995). When linearity of a system performance can be accepted, the principles of superposition and translation in time are applicable. Under the assumption of linear groundwater flow equations (linear boundary conditions and transmissivity values that do not depend on the hydraulic head), influence functions, discrete kernels or response matrices have been applied to embed distributed-parameter simulation of aquifers into conjunctive use management models (Maddock, 1972; Schwarz, 1976, Morel-Seytoux and Daly, 1975). The main advantage of response matrices is their condensed representation of external simulation models. The response functions are incorporated into constraints, coupling the hydrologic simulation with the management optimization. Gorelick et al. (1979) and Gorelick and Remson (1982) first applied a response matrix approach in the development of a management model of a groundwater system with a transient pollutant source.

To apply superposition, we need to assume linearity of the system with regard to the decision variables. For this purpose, in the application of the response matrix approach to groundwater pollution problems, groundwater flow has to be considered as steady state, while nitrate transport can be simulated as time dependent (transient) (Gorelick et al., 1979).

Consistently with the steady state assumption, we assume that each crop area provides a constant recharge to the aquifer and therefore, the groundwater velocity field is time invariant. The concentration recharge is the quotient of the amount of nitrate leaching over the volume of water recharge. Treating both factors as unknowns would create a non-linearity with respect to the advective and dispersive transport, both of which depends on concentration and velocity. To overcome this, groundwater recharge is considered as constant in time. The use of the steady state flow assumption may not be suitable for sites with significant hydraulic head variations in time, because of the transport simulation errors introduced by ignoring flow transient

Nitrate fate and transport and groundwater flow

Solute transport and fate in groundwater depends on the velocity of groundwater flow, which can be obtained solving the groundwater flow equation for steady-state flow through a saturated anisotropic porous medium (Freeze and Cherry, 1979):

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y \frac{\partial H}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z \frac{\partial H}{\partial z}\right)+W=0 \qquad (4)$$

where K_x, K_y and K_z are the hydraulic conductivity values (L/T) in the x, y and z directions; H is the hydraulic head (L) and W is the flux term (L/T) that accounts for pumping, recharge or other sources and sinks.

The solute concentration throughout the aquifer can be described by the general equation for advective-dispersive transport, incorporating equilibrium-controlled sorption and first-order irreversible reactions (Zheng and Bennett, 2002):

$$R\frac{\partial C}{\partial t}=\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right)-\frac{\partial}{\partial x_i}\left(v_i C\right)+\frac{q_s}{\theta}C_s-\lambda\left(C+\frac{\rho_b}{\theta}\overline{C}\right) \qquad (5)$$

where C is the dissolved concentration (M/L^3); t is the time (T); $\overline{C}$ is the sorbed concentration (M/ L^3); v_i is the pore water velocity (L/T); q_s is the volumetric flow rate per unit volume of aquifer and represents fluid sources and sinks (T^{-1}); C_s is the concentration of the fluid sources or sink flux (M/L^3); λ is the reaction rate constant (T^{-1}); ρ_b is the bulk density of the porous medium (M/L^3); θ is the porosity (dimensionless); and R is the retardation factor.

Pollutant Concentration Response Matrix

The response matrix describes the influence of pollutant sources upon concentrations at the control sites over time. Dynamic management of pollutant sources affecting groundwater quality has been examined by Gorelick et al. (1979), Gorelick and Remson (1982), Gorelick (1982) or Ahlfeld (1988). The pollutant concentration response matrix *[RM]* is a rectangular (m x n) matrix. The number of columns, n, equals the number of crop areas (pollution sources) times the number of years within the planning horizon. The number of rows, m, equals the number of control sites times the number of simulated time steps in the frame of the problem (Fig 3). The simulated time horizon corresponds to the time for the solute to pass all the control sites, and it is independent of the length of the planning period.

Sources x Planning horizons

Control sites x Time

	$S_{1,1}$	$S_{2,1}$	…	$S_{s,1}$	$S_{1,2}$	$S_{2,2}$	…	$S_{s,2}$	…	$S_{s,m}$
$O_{1,1}$	$C_{1,1,1,1}$	$C_{1,1,2,1}$		$C_{1,1,s,1}$	$C_{1,1,1,2}$	$C_{1,1,2,2}$		$C_{1,1,s,2}$		$C_{1,1,s,m}$
$O_{2,1}$	$C_{1,2,1,1}$	$C_{1,2,2,1}$		$C_{1,2,s,1}$	$C_{1,2,1,2}$	$C_{1,2,2,2}$		$C_{1,2,s,2}$		$C_{1,2,s,m}$
⋮	⋮	⋮		⋮	⋮	⋮		⋮		⋮
$O_{c,1}$	$C_{1,t,1,1}$	$C_{1,t,2,1}$		$C_{1,t,s,1}$	$C_{1,t,1,2}$	$C_{1,t,2,2}$		$C_{1,t,s,2}$		$C_{1,t,s,m}$
$O_{1,2}$	$C_{2,1,1,1}$	$C_{2,1,2,1}$		$C_{2,1,s,1}$	$C_{2,1,1,2}$	$C_{2,1,2,2}$		$C_{2,1,s,2}$		$C_{2,1,s,m}$
$O_{2,2}$	$C_{2,2,1,1}$	$C_{2,2,2,1}$		$C_{2,2,s,1}$	$C_{2,2,1,2}$	$C_{2,2,2,2}$		$C_{2,2,s,2}$		$C_{2,2,s,m}$
⋮	⋮	⋮		⋮	⋮	⋮		⋮		⋮
$O_{c,2}$	$C_{2,t,1,1}$	$C_{2,t,2,1}$		$C_{2,t,s,1}$	$C_{2,t,1,2}$	$C_{2,t,2,2}$		$C_{2,t,s,2}$		$C_{2,t,s,m}$
⋮	⋮	⋮		⋮	⋮	⋮		⋮		⋮
$O_{c,t}$	$C_{o,t,1,1}$	$C_{o,t,2,1}$		$C_{o,t,s,1}$	$C_{o,t,1,2}$	$C_{o,t,2,2}$		$C_{o,t,s,2}$		$C_{o,t,s,m}$

Fig. 3. Schematic representation of the pollutant concentration response matrix.

Numerical simulation models based on the flow and solute transport governing equations were used to develop the pollutant concentration response matrix. MODFLOW (Mcdonald and Harbough, 1988), a 3D finite difference groundwater flow model, and MT3DMS (Zheng and Wang, 1999), a 3D solute transport model, were applied to ensemble the pollutant response matrix. First, the field of groundwater velocities is computed using the calibrated groundwater flow model. With the velocity field and the calibrated mass transport model, MT3DMS computes the nitrate concentrations over time (breakthrough curve) at each control site resulting from unit nitrate concentration recharges at each pollution source. These concentration values are assembled as columns to conform the pollutant concentration response matrix.

For advection-dominated problems, the solution of the transport equation presents two types of numerical problems: numerical dispersion and artificial oscillations (Zheng and Bennett, 2002). The MT3DMS has several solution techniques, the one used here is the third-order TVD scheme based on the ULTIMATE algorithm which is mass conservative, without excessive numerical dispersion, and essentially oscillation-free (Zheng and Wang, 1999).

Agronomic simulation

Crop production and nitrogen leaching functions can be derived from agronomic simulation models like EPIC (Williams, 1995; Liu et al., 2007). GLEAMS (Knisel et al., 1995; De Paz and Ramos, 2004) and NLEAP (Shaffer et al., 1991; Shaffer et al., 2008) are also popular models for simulating nitrate leaching. In EPIC, a crop growth /chemical transport simulation model help defines functions relating crop yield, and groundwater nitrate leaching to water applied, on-ground nitrogen fertilization and nitrogen stock in the soil. These functions will depend on local conditions on soils, climate, irrigation water, tillage, and other operations.

The crop yield can be defined through crop production functions with the following polynomial equation:

$$Y_c = a + b \cdot W_c + c \cdot W_c^2 + d \cdot N_c + e \cdot N_c^2 + f \cdot W_c \cdot N_c \tag{6}$$

where Y_c is the crop yield (kg/ha), W_c is the water applied to the crop (m^3/ha) and N_c is the fertilizer applied to the crop (kg/ha). Flexible quadratic function forms are often used to characterize crop yields (Doorenbos and Kassam, 1979; Vaux and Pruitt, 1983; Zhengfei et al., 2006). The coefficients of the equation (a, b, c, d, e, and f) are calibrated for the best fit to the values obtained through an external agronomic simulation model.

The amount of leaching and hence the amount of nitrates in groundwater is a function of the timing of fertilizer application, vegetative cover, soil porosity, fertilizer application method, and irrigation rate (Canter, 1996). After the plant uptake and transformation, some of that nitrogen applied is converted into nitrate that can leach to the aquifer. The amount of nitrate leached is then introduced into the management model through quadratic functions of water applied and nitrogen fertilization, also this functions are often used to characterize nitrate leaching (Calatrava and Garrido, 2001; Martinez and Albiac, 2004;) as follows:

$$L_c = g + h \cdot W_c + i \cdot W_c^2 + j \cdot N_c + k \cdot N_c^2 + l \cdot W_c \cdot N_c \quad (7)$$

where L_c is the nitrogen leached (kg/ha), W_c is the water applied to the crop (m^3/ha) and N_c is the fertilizer applied to the crop (kg/ha). The coefficients of the equation (g, h, i, j, k, and l) are calibrated for the best fit to the values obtained through an external agronomic simulation model.

APPLICATION OF THE MODELLING FRAMEWORK

Illustrative example

The modelling framework was applied to a hypothetical groundwater system (Fig. 4). The aquifer has impermeable boundaries and steady flow from the top to bottom of the Figure. The finite difference grid is 500 x 500 meters. The system parameters are hydraulic conductivity of 40 m/day, aquifer thickness of 10 meters, effective porosity of 0.2, and dispersivity of 10 meters. The natural recharge is 500 m^3/ha. There are 70 stress periods, each of one year (365 days). Seven crop zones with five different crops are considered. For each crop a quadratic production function and a leaching function have been defined. Each source is related to a crop as shown in Figure 4. The coefficients used for the production and nitrate leaching functions are shown in Table 1. Three control sites with concentration upper bounds (maximum of 50 mg/l of nitrates) are defined.

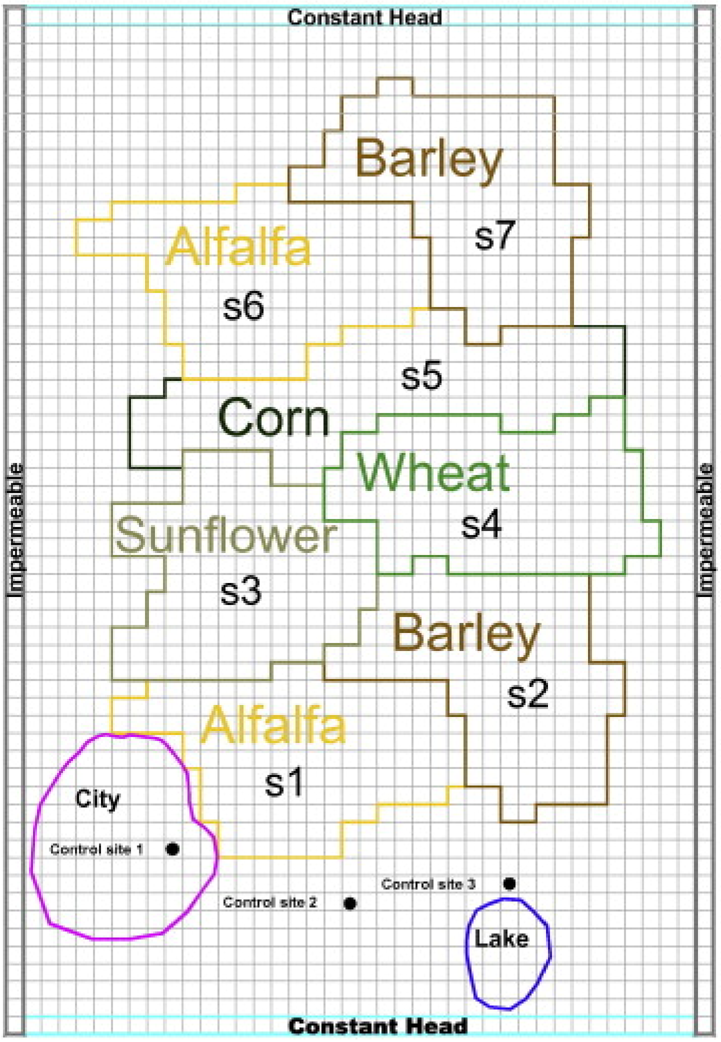

Fig. 4. Aquifer system

Table 1
Production function and nitrogen leaching coefficients.

Crop	a	b	c	d	e	f
Production functions coefficients						
Alfalfa	4.43E+00	2.63E−02	−1.62E−05	4.68E−02	−3.45E−04	0.00E+00
Barley	−3.68E−01	6.06E−03	−1.02E−05	1.88E−02	−5.15E−05	0.00E+00
Sunflower	4.37E−01	6.80E−04	−9.70E−06	3.12E−02	−1.40E−04	5.40E−05
Wheat	6.11E−01	3.90E−03	−3.40E−05	4.60E−02	−1.30E−04	5.00E−05
Corn	−1.30E+01	3.80E−02	−2.40E−05	6.70E−03	−7.20E−05	5.17E−05
	g	h	i	j	k	l
Leaching functions coefficients						
Alfalfa	−7.04E+00	−3.69E−03	1.36E−05	9.69E−03	1.02E−03	0.00E+00
Barley	−1.96E+01	−1.15E−03	2.20E−04	−2.04E−02	5.06E−04	0.00E+00
Sunflower	0.00E+00	0.00E+00	−3.44E−04	7.68E−01	−2.25E−03	1.34E−03
Wheat	0.00E+00	4.36E−02	0.00E+00	3.05E−01	1.30E−04	−1.17E−04
Corn	0.00E+00	4.40E−03	−6.69E−05	3.96E−01	0.00E+00	0.00E+00

Table 2
Sources, crops and irrigation.

Source	Crop	Area (ha)	Water applied (m^3/ha)	Crop price (€/kg)
S1	Alfalfa	3600	950	0.09
S2	Barley	3600	300	0.12
S3	Sunflower	3600	400	0.30
S4	Wheat	3600	250	0.13
S5	Corn	3600	700	0.12

The irrigation water applied was kept constant at the level where the crop yield is maximum (Table 2). The fertilizer price is 0.60 €/kg.

Pollutant concentration response matrix and breakthrough curves

The response matrix is generated by simulating the effects of a fertilizer application of 200 Kg/ha and an annual recharge of 500 m^3/ha. Using the corresponding concentration recharge as "unit" recharge rate at each source, the breakthrough curves (nitrate concentration time series) for the different sources were generated using MODFLOW and MT3DMS. For the solute transport simulation only advection and dispersion were considered, and the simulation time horizons were determined by the time for which the solute completely passed the control sites. Breakthrough curves were obtained for each crop area and for the three different control sites (Fig. 5).

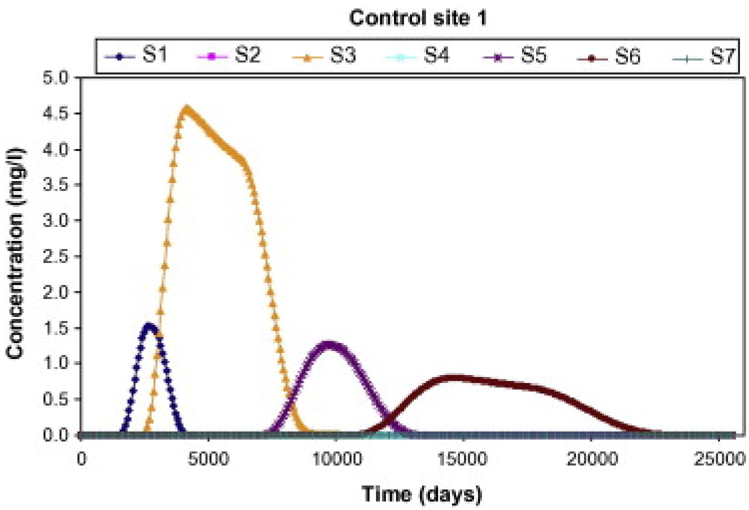

Fig. 5. Breakthrough curve for the control site 1.

Crop area S3 (sunflower) is the nitrate source with the greatest influence on control sites 1 and 2, followed by *S1.* Source *S3* has greater influence than sources *S1* and *S2*, despite these areas are closer to the control sites (Fig. 4), since nitrate leaching concentration from S3 is higher than from the other crop areas. *S5* (corn) is the only pollution source with a significant impact on the three control sites.

Scenarios and results

Five different scenarios have been considered to illustrate the applicability of the proposed approach. In the scenario 0 or base case, no ambient standards are considered, and the fertilizer applied is the one that yields the highest benefit. In scenarios 1 to 4, a maximum nitrate concentration of 50 mg/l is imposed at the three control sites as follows:

- Scenario 1. The initial solute concentration in groundwater is zero, and the fertilizer application can vary in space and time.
- Scenario 2. The initial solute concentration in groundwater is zero and the fertilizer application is restricted to be the same over the planning horizon.
- Scenario 3. The initial solute concentration is 55 mg/l throughout the aquifer, and the fertilizer application can vary in time and space. For this scenario four different recovery times were considered: 10, 20, 30 and 40 years.
- Scenario 4. The initial concentration is 55 mg/l and the fertilizer application is restricted to be the same for all the management periods.

For each scenario, four planning horizons (10, 20, 30 and 40 years) were considered to test the influence of the planning horizon on the optimal nitrate management and its economic and environmental impacts.

The model was coded in GAMS, a high-level modelling system for mathematical programming problems (GAMS, 2008). The non-linear problem to be solved has 1681 variables and 2939 constraints. The MINOS solver was used to find the optimal solution.

Scenario 0. No nitrate standard

This scenario is a reference case with no nitrate standard and the aquifer not initially polluted. Therefore, the resulting fertilizer application is the one that yields the maximum aggregated net benefit, without constraining nitrate pollution. The optimal fertilizer distribution in space and time was calculated for 10, 20, 30 and 40 year planning horizons. The longer the considered planning horizon, the higher the peak concentration of nitrate.

While for the 10 year planning horizon the maximum concentration is below the current standard, the nitrate standard is exceeded for 20 year and longer planning horizons (64 mg/l would be reached in the 40 year planning horizon case). Since in all the planning horizons the optimal fertilizer application would be the same (3731 ton/year on average), an equal annual benefit (20.96 M€/year) would be obtained.

Scenario 1. Variable fertilizer application.

For the 10 year planning horizon, the fertilizer application was the same as that providing the maximum benefits, since the ambient standard was not reached at any of the control sites. However, for longer planning horizons (20, 30, and 40 years) the fertilizer application was reduced to keep nitrate concentrations at the control sites below 50 mg/l. Figure 6 shows the optimal fertilizer application for the different planning horizons, showing the application is further reduced as the planning horizon increases, since there is an extension in time of the application of the fertilizer loading. From here on, only the results for the 40 year management period will be shown, a representing long-term management.

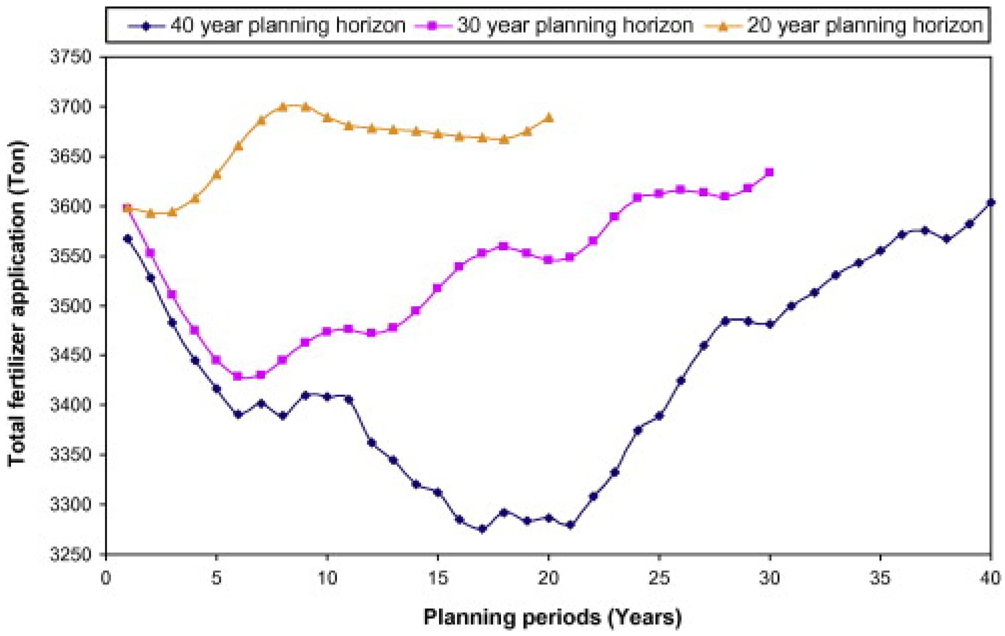

Fig. 6. Total fertilizer application for different planning horizons. Scenario 1.

Figure 7 shows the reduction of fertilizer application corresponding to each source with regards to the fertilizer application of maximum crop yield. The level of sustainable fertilizer loading reduction differs with location depending on its influence upon the nitrate concentration at the control sites and the economic losses from crop yield reduction. According to this Figure, crop area *S5* (corn) requires the most fertilizer reduction, reaching a 30% reduction during the first 30 years. As shown in Figure 5, this crop area strongly influences nitrate concentration at the 3 sites.

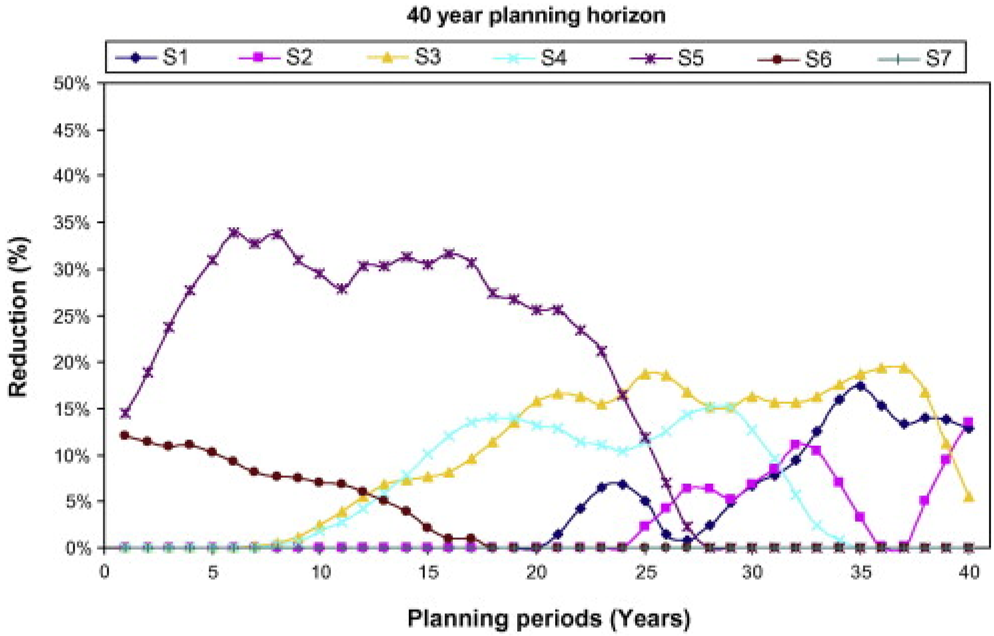

Fig 7. Spatial and temporal reduction of fertilizer application. Scenario 1.

The arrival time of the peak nitrate concentration to the control sites differs for each source; therefore, the optimal timing and magnitude of fertilizer reduction to meet the environmental targets will differ for each source. Figure 8 shows the times series of nitrate concentration for the optimal fertilizer application at the 3 control sites. Figure 8 shows that nitrate concentrations are maintained below the ambient standard of 50 mg/l. While the concentrations at control site 1 and 2 are close to the limit, the values at control site 3 are notably below.

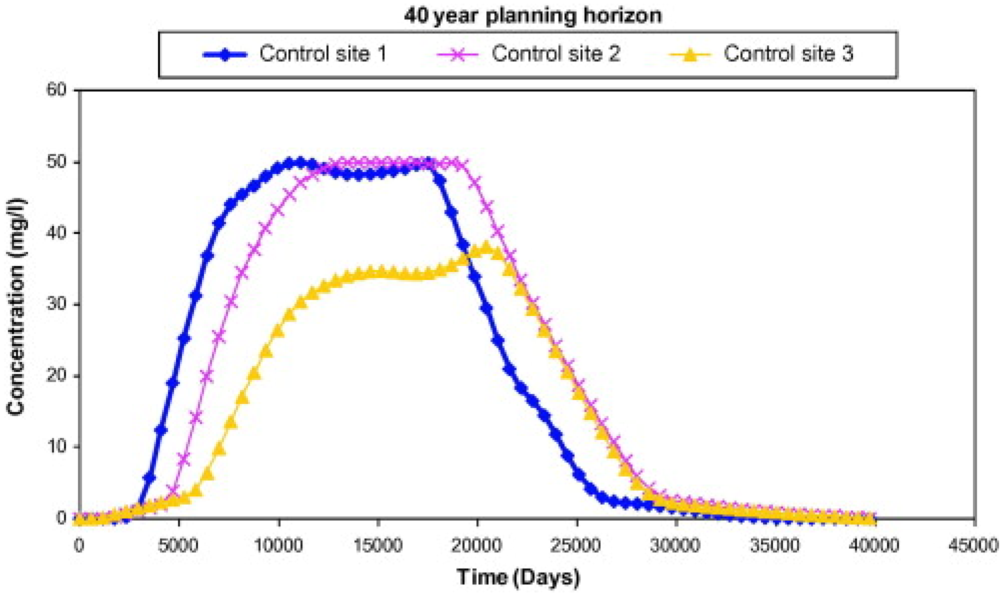

Fig. 8. Time series of nitrate concentration. Scenario 1.

Table 3 shows the economic impacts of different planning horizons. The longer the planning horizon, the higher the reduction in fertilizer application, with lower average benefits per year.

Table 3
Fertilizer application and benefit for different planning horizons. Scenario 1.

Planning horizon (years)	Total annual fertilizer application (ton/year)	Total benefit (M€/year)
10	3731	20.96
20	3660	20.93
30	3533	20.83
40	3429	20.76

Scenario 2. Constant fertilizer application.

Scenario 2 illustrates the case where the fertilizer application is kept constant through the years, which is obviously not the economically optimal solution but represents a simpler management alternative. Table 4 shows the fertilizer application and the percentage of fertilizer reduction from the loading that produces the maximum crop yield that is required to meet the ambient standards. Crop area *S5* (corn) again has the highest fertilizer reduction, followed by *S3* (sunflower).

Table 4
Constant fertilizer application and percentage of fertilizer reduction. Scenario 2.

Source	Crop	Fertilizer application (kg/ha)	Fertilizer reduction (%)
S1	Alfalfa	50.1	13.9
S2	Barley	124.1	7.5
S3	Sunflower	151.9	16.2
S4	Wheat	180.3	13.0
S5	Corn	183.7	30.2
S6	Alfalfa	55.8	4.1
S7	Barley	134.1	0.0

Comparing the fertilizer application in scenarios 1 and 2 (Fig. 9) we conclude that when the fertilizer application is constant over time (scenario 2) the total fertilizer application has to be reduced to meet the constraints. Over time, both curves get closer up to the point in which the minimal fertilizer application in scenario 1 reaches the value in scenario 2. Since scenario 2 presents the highest reductions in fertilizer applications, the benefits for agriculture are consequently lower (20.50 against 20.96 M€/year).

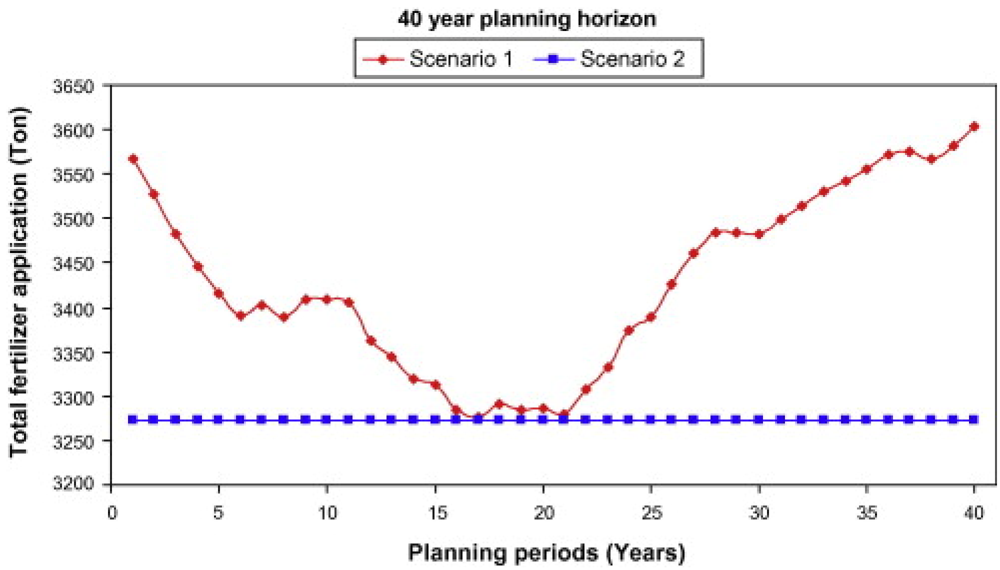

Fig. 9. Comparison between scenarios 1 and 2.

Scenario 3. Recovery from pollution.

The EU Water Framework Directive requires determining the most cost-efficient combination of measures to reduce nitrate concentration in polluted groundwater bodies below the standard (50 mg/l). In this scenario, an initial uniform nitrate concentration of 55 mg/l was considered, and the objective was to find the optimal fertilizer application to reduce nitrate groundwater concentrations to 50 mg/l for different recovery time horizons (10, 20, 30 and 40 years). The recovery time horizons were imposed in the management model by setting the maximum concentration constraint at the specific recovery time and beyond.

Figure 10 shows the fertilizer application for the scenarios 1 (initially unpolluted aquifer) and 3 (initially polluted aquifer) with a 40 year recovery time horizon. The fertilizer application is higher for scenario 1 than for scenario 3 to reduce the initial nitrate concentrations. However, both applications converge over time, once the effect of the initial concentration has been lowered by natural attenuation.

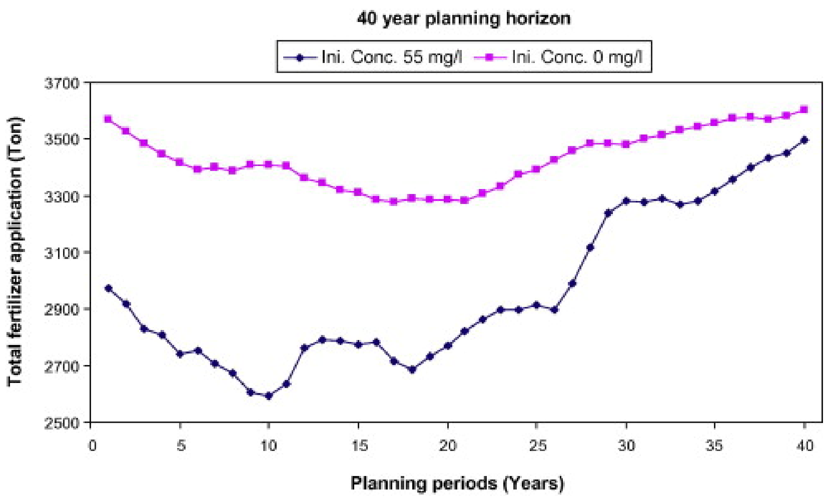

Fig. 10. Comparison between scenarios 1 and 3.

Table 5 shows the benefits for the different recovery times. The difference in benefits between the more constrained case (10 year recovery time) and the 40 years of recovery is €230,000/year.

Table 5
Total benefits for different recovery times. Scenario 3.

Recovery time (years)	Total fertilizer application (ton/year)	Total annual benefits (M€/year)
10	2898	19.43
20	2917	19.45
30	2921	19.53
40	2964	19.66

Figure 11 depicts the total fertilizer application that corresponds to the different recovery time horizons.

Longer recovery time horizons increase total fertilizer application (concentrations must be reduced faster for shorter recovery times). However, the differences decrease over time.

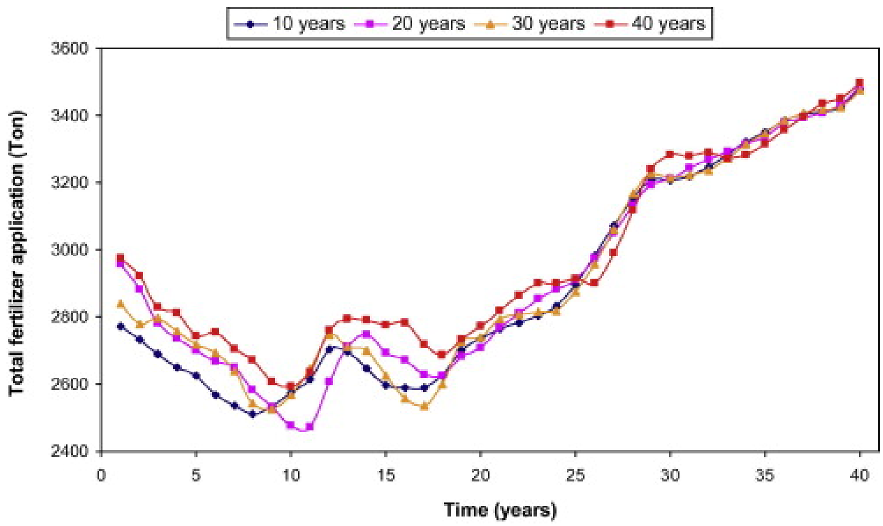

Fig 11. Total fertilizer application for different recovery times. 40 year planning horizon. Scenario 3.

Scenario 4. Constant fertilizer application with initial pollution.

In this scenario the aquifer is considered polluted with an initial uniform concentration of 55 mg/l, and the fertilizer application is kept the same throughout the planning horizon.

Comparing scenarios 3 and 4 for the 40 year planning period case, there is a significant reduction in the benefits from agriculture (€580,000/year) when the fertilizer is kept constant, although the difference in the average fertilizer application is only 15 kg/ha-year.

Some researchers (e.g., Yadav, 1997; Martinez and Albiac, 2004) have performed cost-effectiveness analysis of groundwater pollution control policies as if the ambient standards were imposed at every location in the aquifer, and therefore, the pollutant concentration recharge is implicitly limited to 50 mg/l. The same case was simulated and compared with the results previously obtained imposing nitrate concentration limits only at the three control sites. Table 6 shows the total fertilizer reduction required for maintaining nitrate concentration below 50 mg/l throughout the aquifer, showing that no fertilizer reductions are required for some crops, since the quantity of fertilizer that yields the highest crop production can be applied without exceeding the ambient standard. However, other crops (sunflower, wheat, corn) require a big reduction in fertilizer loads. With these fertilizer application rates, the maximum nitrate concentration at the control points stays below 20 mg/l, far from the limit of 50 mg/l. Because of the further reduction in fertilizer application, the average benefits are considerable smaller (17.09 M€/year versus 19.08 M€/year).

Table 6
Fertilizer application and fertilizer reduction for the case where the concentration recharge is below 50 mg/l.

Source	Crop	Fertilizer application (kg/ha)	Fertilizer reduction (%)
S1	Alfalfa	58.2	0
S2	Barley	134.1	0
S3	Sunflower	69.8	62
S4	Wheat	50.0	76
S5	Corn	138.1	48
S6	Alfalfa	58.2	0
S7	Barley	134.1	0

CONCLUSIONS

In recent decades, nitrate concentrations in groundwater have increased due to the intensive use of fertilizers in agriculture. In Europe, the EU water legislation establishes a limit of nitrate concentration in groundwater bodies of 50 mg/l, and requires that groundwater bodies reach a good quantitative and chemical status by 2015. To control groundwater diffuse pollution is necessary to analyse and implement management decisions.

This paper describes the development and application of a method for exploring optimal management of groundwater nitrate pollution from agriculture. The model suggests the spatial and temporal fertilizer application rate that maximizes the net benefits in agriculture constrained by the quality requirements in groundwater at specific control sites. The analysis accounts for key underlying biophysical processes linked to the dynamics of nitrogen in the soil and the aquifer, as well as the crop yield responses to water and fertilizer application. External soil-plant agronomic models, and groundwater flow and solute transport simulation models are used to obtain influence or response functions that are integrated into the optimization model, translating nitrogen applied on the surface into nitrates at wells or other points of interest throughout the aquifer, so the effectiveness of measures can be assessed in terms of reduction of nitrate concentrations within the groundwater body. Unlike simulation approaches, the management model automatically generates optimal solutions for a very complex problem. Instead of resorting to black-box statistical models, the fate and transport of nitrates within the aquifer is explicitly simulated in the optimization model using a pollutant concentration response matrix under the assumption of steady-state flow. The concentration response matrix shows the concentration over time at different control sites throughout the aquifer resulting from multiple pollutant sources distributed over time and space.

The method was applied to an example under five scenarios. Optimal solutions to problems with different initial conditions, planning horizons and recovery times were found. The case study shows how both the selected planning horizon and the target recovery time can strongly influence the limitation of fertilizer use and the economic opportunity cost for reaching the environmental standards. There is clearly a trade-off between the time horizon to reach the standards (recovery time) and the economic losses from nitrogen use reductions.

This method can contribute to implementing the EU Water Framework Directive by providing insights for the definition of cost-efficient policies or program of measures to control diffuse groundwater pollution. The modelling framework allows estimation of the opportunity cost of measures to reduce nitrogen loadings and their effectiveness for maintaining groundwater nitrate concentration within the target levels. The method also can be applied to identifying economically efficient “good quality status” threshold values. Finally, it can be used to justify less stringent environmental objectives based on the existence of disproportionate cost (for cases in which opportunity costs surpass the expected benefits) or to ask for deadline extensions when it is not feasible or the objectives cannot “reasonably” be achieved within the required timescales.

Additional work to assess the influence of uncertainty in the different parameters of the model would be required. A stochastic modelling framework can be derived from the proposed methodology. The modelling framework can be used to test the effects of different policies such as water prices, nitrogen taxes, nitrogen standards, subsidies, etc. Finally, the method can be extended to consider other sources of nitrate pollution such as animal farming, landfills, and septic tanks. Although the method and tools are suitable for simulating the effects of these sources on nitrate concentration at the control sites, further research would be required for modelling the economics of abating the pollution from these other sources.

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