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

PhD Thesis submitted by

Salvador Peña Haro

Director (advisor):

Manuel A. Pulido Velázquez

Codirector (coadvisor):

David Pulido Velázquez

UNIVERSIDAD POLITECNICA DE VALENCIA

Instituto de Ingeniería del Agua y Medio Ambiente

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Con cariño para Sabina,

por supuesto

“What makes the desert beautiful is that somewhere it hides a well”

Antoine de Saint-Exupery

“When the well is dry, we know the worth of water”

Benjamin Franklin

“Essentially, all models are wrong, but some are useful”

George Edward Pelham Box

Abstract

Diffuse groundwater pollution is a growing concern everywhere in the world and one of the most problematic and widespread of the vast number of potential groundwater contaminants are nitrates, which often primarily comes from the intense use of fertilizer in agriculture.

Groundwater pollution has provoked a normative and a recommendation development. In Europe the Nitrate Directive was established in 1991, and the Water Framework Directive (WFD) in 2000. The WFD states that all water bodies have to reach a good quality status by 2015. The WFD explicitly recognizes the role of economics in reaching environmental and ecological objectives. One of the elements that the WFD mentions is the cost-effectiveness analysis (CEA) as a method to obtain the most cost-effective program of measures to reach good water status.

A hydro-economic modeling framework is developed for determining optimal management of ground water 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 simulation models are used to obtain crop yield and nitrate leaching functions in terms of water and fertilizer use, 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. In this way, this framework provides a practical 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.

In decision-making processes, reliability and risk-aversion play a decisive role. This dissertation presents a stochastic optimization framework to incorporate the effects of the hydraulic conductivity uncertainty on the least-cost allocation of nitrogen reduction among the agriculture pollution sources in order to meet the groundwater nitrate concentration targets in a groundwater basin under heterogeneous physical conditions. Four different formulations were applied: Monte Carlo simulation with pre-assumed parameter field, Monte Carlo optimization, stacking management, and mixed-integer stochastic model with predefined reliability. These formulations were tested in an illustrative example were 100 realizations were performed for two cases with different hydraulic conductivity field variance.

The methodology was applied also to a real case-study, "El Salobral-Los Llanos" (within the Mancha Oriental groundwater body). The model yields the optimal fertilizer application that meets the groundwater nitrate standard for a 50 year planning horizon. The average fertilizer application has to be reduced by 39 kg/ha in order to comply with the environmental standard. This reduction implies a smaller production, which represents a forgone benefit of about 1.2 M€/year.

Despite the necessary limitations of any modeling approach, the relevance and complexity of real-world groundwater diffuse pollution issues call for the development of integrated hydro-economic models in order to address the problem of multiple pollution sources under heterogeneous conditions, integrating the main agronomic, economic and biophysical elements of the process (including the associated uncertainty) at the groundwater basin scale. This research provides a useful methodology and tool for decision-making in the ongoing process of implementation of the Water Framework Directive and the Groundwater Daughter Directive criteria to the groundwater bodies. Further research would be required in order to extend the representation of the diversity of potential on-farm management decisions and other policy options apart from fertilizer use limitations.

Resumen

La contaminación difusa de las aguas subterráneas es una creciente preocupación en cualquier parte del mundo, y los nitratos, principalmente originados por el uso intensivo de fertilizantes en la agricultura, son uno de los contaminantes en el agua subterránea problemáticos y extendidos.

La contaminación de los acuíferos ha provocado el desarrollo de numerosas normativas y recomendaciones. En Europa, la Directiva de Nitratos fue establecida en 1991, y la Directiva Europea Marco del Agua (DMA) en 2000. La DMA establece que todas las masas de agua deben alcanzar el buen estado en el año 2015. La DMA explícitamente reconoce el rol que la economía puede tener el alcanzar los objetivos ecológicos y ambientales. Uno de los elemento que la DMA menciona es el análisis coste-eficacia (ACE), éste análisis puede ser usado para obtener el programa de medidas más coste-eficaz para alcanzar el buen estado de las masas de agua.

En este trabajo se presenta el desarrollo de un modelo hidro-económico para determinar la gestión óptima de la contaminación por nitratos de las agua subterráneas. El modelo holístico de optimización determina la distribución espacio-temporal de la tasa de aplicación de fertilizantes que maximiza los beneficios netos en la agricultura, limitada por los requerimientos de calidad en el agua subterránea en diferentes puntos de control. Dado que las emisiones (cantidad de nitrógeno) son controlables pero los objetivos se refieren a concentraciones, es necesario relacionar ambos aspectos. Mediante modelos de simulación agronómica se obtienen las funciones de producción y de lixiviado de nitratos en función del uso de agua y fertilizantes, mientas que se emplean modelos numéricos de simulación del flujo y transporte para obtener soluciones unitarias que se integraron en el modelo de optimización por medio de matrices de respuesta. La integración de las matrices de respuesta en el modelo de gestión permite simular la evolución de la concentración de nitratos en el agua subterránea mediante superposición en diferentes puntos de control a largo del tiempo, debido a la emisión de contaminantes en diferentes zonas distribuidas en el espacio y variables en el tiempo. De este modo el modelo relaciona la aplicación de fertilizantes con la concentración de nitratos en el agua subterránea. Los beneficios de la agricultura se determinaron a través de las funciones de producción y el precio de los cultivos. De esta forma, se obtiene una herramienta práctica para analizar el coste de oportunidad de medidas para reducir la carga de nitrógeno y evaluar su eficacia para mantener las concentraciones de nitratos en los acuíferos dentro de los niveles fijados como objetivo.

El modelo desarrollado se aplicó a un sistema acuífero sintético. Se obtuvo la aplicación óptima de fertilizantes para problemas con diferentes condiciones iniciales, horizontes de planeación y tiempos de recuperación. Los resultados del caso sintético muestran la importancia de la localización de las fuentes contaminantes en relación con los puntos de control. Los horizontes de planeación y los tiempos de recuperación pueden tener una gran influencia en la aplicación de fertilizantes y en el coste de oportunidad para alcanzar los estándares medioambientales. Hay un claro intercambio entre el horizonte de

planeación para alcanzar los estándares de calidad (tiempo de recuperación) y las pérdidas económicas debidas a la reducción de nitratos en la agricultura.

En el proceso de toma de decisiones, la fiabilidad y la aversión al riesgo juegan un papel importante. Se presenta un modelo de optimización estocástico para la analizar los efectos de la incertidumbre en la conductividad hidráulica sobre la solución de menor coste de la distribución de reducciones en la aplicación de nitrógeno entre las diferentes fuentes de contaminación para alcanzar los objetivos de concentración de nitratos en una masa subterránea heterogénea. Se analizaron cuatro métodos diferentes: simulación Monte Carlo con campo de conductividad pre-definido, optimización Monte Carlo, optimización por grupos y un modelo estocástico con optimización entera mixta y nivel de fiabilidad definido a priori. Los modelos se probaron en el caso sintético con 100 realizaciones y dos casos con diferente varianza en el campo de conductividad.

Finalmente la metodología se aplicó al acuífero "El Salobral-Los Llanos" (en el dominio de la masa subterránea Mancha Oriental), para el que se obtuvo la aplicación óptima de fertilizantes para una horizonte de planeación de 50 años. La aplicación promedio tiene que ser reducida en 39 kg/ha, lo cual provoca una reducción en la producción con un coste (pérdida de beneficios) de 1.2 M€/año.

A pesar de las limitaciones necesarias de cualquier modelo, la relevancia y complejidad de los problemas reales de contaminación difusa de aguas subterráneas requiere el desarrollo de modelos integrales hidro-económicos para resolver el problema de múltiples fuentes de contaminación en condición heterogéneas, integrando los principales elementos agronómicos, biofísicos y económicos del proceso (incluyendo la incertidumbre) a escala de masa de agua subterránea. De esta forma, el trabajo desarrollado proporciona una metodología y unas herramientas que pueden ser de utilidad para la toma de decisiones en el proceso de implementación de los requerimientos de la Directiva Marco y la reciente Directiva Hija de protección de Aguas Subterráneas frente a la contaminación. Una línea de trabajo futura sería ampliar la diversidad de decisiones de gestión en parcelas y otras opciones de política de control, aparte de las de limitación en el uso de fertilizantes.

Resum

La contaminació difusa de les aigües subterrànies és una creixent preocupació en qualsevol part del món, i els nitrats, principalment originats per l'ús intensiu de fertilitzants en l'agricultura, són un dels contaminants en l'aigua subterrània problemàtics i estesos.

La contaminació dels aqüífers ha provocat el desenrotllament de nombroses normatives i recomanacions. A Europa, la Directiva de Nitrats va ser establida en 1991, i la Directiva Europea Marco de l'Aigua (DMA) en 2000. La DMA establix que totes les masses d'aigua han d'aconseguir el bon estat l'any 2015. La DMA explícitament reconeix el rol que l'economia pot tindre l'assolir els objectius ecològics i ambientals. Un dels element que la DMA menciona és l'anàlisi cost-eficàcia (ACE), esta anàlisi pot ser usat per a obtindre el programa de mesures més cost-eficaç per a aconseguir el bon estat de les masses d'aigua.

En este treball es presenta el desenrotllament d'un model hidro-económico per a determinar la gestió òptim de la contaminació per nitrats de les aigua subterrànies. El model holístic d'optimització determina la distribució espai-temporal de la taxa d'aplicació de fertilitzants que maximitza els beneficis nets en l'agricultura, limitada pels requeriments de qualitat en l'aigua subterrània en diferents punts de control. Atés que les emissions (quantitat de nitrogen) són el controlable però els objectius són les concentracions, és necessari relacionar ambdós aspectes. Per mitjà de models de simulació agronòmica es obtenen les funcions de producció i de lixiviat de nitrats en funció de l'ús d'aigua i fertilitzants, esmentes que s'empren models numèrics de simulació del flux i transport per a obtindre solucions unitàries que es van integrar en el model d'optimització per mitjà de matrius de resposta. La integració de les matrius de resposta en el model de gestió permet simular l'evolució de les concentració de nitrats en l'aigua subterrània per mitjà de superposició en diferents punts de control a llarg del temps, resultat de l'emissió de contaminants en diferents zones distribuïdes en l'espai i variables en el temps. D'esta manera el model relaciona l'aplicació de fertilitzants amb la concentració de nitrats en l'aigua subterrània. Els beneficis de l'agricultura es van determinar a través de les funcions de producció i el preu dels cultius. D'esta manera, s'obté una ferramenta pràctica per a analitzar el cost d'oportunitat de mesures per a reduir la càrrega de nitrogen i avaluar la seua eficàcia per a mantindre les concentracions de nitrats en els aqüífers dins dels nivells objectiu.

El model desenrotllat es va aplicar a un sistema aqüífer sintètic. Es va obtindre l'aplicació òptima de fertilitzants per a problemes amb diferents condicions inicials, horitzons de planeación i temps de recuperació. Els resultats del cas sintètic mostren la importància de la localització de les fonts contaminants en relació amb els punts de control. Els horitzons de planeación i els temps de recuperació poden tindre una gran influència en l'aplicació de fertilitzants i en el cost d'oportunitat per a aconseguir els estàndards mediambientals. Hi ha un clar intercanvi entre l'horitzó de planeación per a aconseguir els estàndards de qualitat (temps de recuperació) i les pèrdues econòmiques degudes a la reducció de nitrats en l'agricultura.

En el procés de presa de decisions, la fiabilitat i l'aversió al risc juguen un paper important. Es presenta un model d'optimització estocástico per a l'analitzar els efectes de la incertesa en la conductivitat hidràulica sobre la solució de menor cost de la distribució de reduccions en l'aplicació de nitrogen entre les diferents fonts de contaminació per a assolir els objectius de concentració de nitrats en una massa subterrània heterogènia. Es van analitzar quatre mètodes diferents: simulació Muntanya Carlo amb camp de conductivitat predefinit, optimització Monte Carlo, optimització per grups i un model estocástico amb optimització sencera mixta i nivell de fiabilitat definit a priori. Els models es van provar en el cas sintètic amb 100 realitzacions i dos casos amb diferent varianza en el camp de conductivitat.

Finalment la metodologia es va aplicar a l'aqüífer "El Salobral-Los Plans" (en el domini de la massa subterrània Manxa Oriental), per al que es va obtindre l'aplicació òptima de fertilitzants per a una horitzó de planeación de 50 anys. L'aplicació mitjana ha de ser reduïda en 39 kg/ha, la qual cosa provoca una reducció en la producció amb un cost (pèrdua de beneficis) de 1.2 €/M'any.

A pesar de les limitacions necessàries de qualsevol model, la rellevància i complexitat dels problemes reals de contaminació difusa d'aigües subterrànies requerix el desenrotllament de models integrals hidro-económicos per a resoldre el problema de múltiples fonts de contaminació en condició heterogènies, integrant els principals elements agronòmics, biofísics i econòmics del procés (incloent la incertesa) a escala de massa d'aigua subterrània. D'esta manera, el treball desenrotllat proporciona una metodologia i unes ferramentes que poden ser d'utilitat per a la presa de decisions en el procés d'implementació dels requeriments de la Directiva Marco i la recent Directiva Filla d'Aigües Subterrànies a les masses subterrànies. Una línia de treball futura seria estendre la representació de la diversitat de decisions de gestió en parcel·la i altres opcions de política de control, a banda de les de limitació en l'ús de fertilitzants.

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Publications

The following publications were done from this thesis:

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S. Peña-Haro, C. Llopis-Albert, M. Pulido-Velazquez. Stochastic hydro-economic modeling for optimal management of groundwater nitrate pollution under parameter uncertainty. *Water Resources Research*. Under review

S. Peña-Haro, C. Llopis-Albert, M. Pulido-Velazquez, D. Pulido-Velazquez. Fertilizer standards for controlling nitrate pollution in groundwater. El Salobral-Los Llanos case study. Submitted to the *Journal of Hydrology*.

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1 General context

1.1 Motivation and objectives

Water pollution is one of the biggest environmental problems and 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). These activities pollute superficial water courses as well as groundwater through percolation. The fertilizers deteriorate the water quality inducing economical and ecological problems. In the last century automation of agriculture and the introduction of high yield crops has raised the use of fertilizers, increasing nitrate concentration in groundwater.

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.

The nitrogen average fertilizer use in Europe is 70 kg/ha (EEA, 2003). In some regions with irrigation-intensive agriculture such as the Mediterranean coast, Castilla-La Mancha region and the Ebro and Guadalquivir basins, the water bodies reach nitrate concentrations between 50-100 mg/l (Martinez and Albiac, 2004). The monitoring networks in the EU indicate that about 20% of groundwater suffers nitrates concentration over 50 mg/l, and 40% over 25 mg/l. Nitrogen from agricultural sources accounts for between 50 and 80% of the nitrates entering Europe's water (EC, 2002).

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. 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/ 92 118/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).

The European Commission (EC, 2002) mentions that the Member States are facing difficulties in preparing forecast of the Action Programmes and the water quality, highlighting the need of "prediction tools that can assess the impact of the preventing measures". Reliable and practical models will be required to correlate the main steps and factors. The effects of most measures are currently evaluated in terms of their emission reduction potential, not their impact in water quality measured through the change in pollutant concentration levels basin-wide, these models should address this issue. In the other hand, it is important to ensure that public funds are allocated to measures and regions according to their potential in solving nitrate losses and eutrophication problems. It is thus important to compare the costs of different measures or programmes to their impact or effectiveness, in reducing drinking water or eutrophication problems (EC, 2002).

The objective of this study is to develop a hydro-economic modeling framework for optimal management of groundwater nitrate pollution from agriculture that suggests the optimal fertilizer application that maximizes the benefits in agriculture while maintaining the nitrate concentrations in groundwater below a target limit. The optimization modeling framework explicitly integrates nitrate leaching and fate and transport in groundwater with the economic impacts of nitrogen fertilizer restrictions in agriculture. Thereby, the on-ground loadings are related to the nitrate concentrations in groundwater. Moreover, a stochastic framework was implemented to incorporate the uncertainty in the conductivity field into the management model, and to analyze the reliability in the optimal strategy designed. 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 (the first one, to be established by 2012), as well as in providing a methodology for assessing the efficiency of different management strategies to reduce nitrate concentrations in groundwater, like land use policies, fertilizer prices and fertilizer standards.

1.2 Legislation on groundwater nitrate pollution

Water pollution has given rise to the development of an extensive legal framework. The focus of this review will be on the EU legislation related to groundwater nitrate pollution. In the European Union, the Nitrates Directive (Directive 91/676/EEC) was established in 1991, the Drinking Water Directive (80/778/EEC and its revision 98/83/EC) in 1998, and the EU Water Framework Directive (Directive 2000/60/EC; WFD) in 2000. The Groundwater Daughter Directive (Directive 2006/118/EC) was enacted in 2006 to complement some articles of the WFD with the aim of preventing and controlling groundwater pollution.

<u>Nitrates Directive</u>

In the 80's there was an increment in livestock farming and in intensive crop-growing involving chemicals and fertilization, which result in an increment of nitrate concentration in water. The Frankfurt Ministerial Conference of 1988 examined water protection legislation, and stressed the need for improving it; this resulted in the adoption of the Directive on urban waste water and the Directive on nitrates[1].

The nitrate directive (91/676/EEC) was adopted in 1991 with the objective of reducing water pollution caused by nitrates from agricultural sources and preventing further such pollution. The Nitrates Directive obliges member states to designate

[1] http://europa.eu/scadplus/leg/en/lvb/l28013.htm

vulnerable zones[2], and to establish and implement Action Programmes. Also, member states shall draw up and implement suitable monitoring programmes to assess the effectiveness of action programmes. The Nitrate Directive suggests two strategies to decrease nitrate pollution: the Codes of Good Agricultural Practice, to be implemented by farmers on a voluntary basis, and the Action programmes in designated areas.

The Codes of Good Agricultural Practice considers (Annex II);

- *Periods when the land application of fertilizer is inappropriate.*
- *The land application of fertilizer to steeply sloping ground.*
- *The land application of fertilizer to water-saturated, flooded, frozen or snow-covered ground.*
- *The conditions for land application of fertilizer near water courses.*
- *The capacity and construction of storage vessels for livestock manures, including measures to prevent water pollution by run-off and seepage into the groundwater and surface water of liquids containing livestock manures and effluents from stored plant materials such as silage.*
- *Procedures for the land application, including rate and uniformity of spreading, of both chemical fertilizer and livestock manure, which will maintain nutrient losses to water at an acceptable level.*

Member States may also include in their code(s) of good agricultural practices the following items:

- *Land use management, including the use of crop rotation systems and the proportion of the land area devoted to permanent crops relative to annual tillage crops.*
- *The maintenance of a minimum quantity of vegetation cover during (rainy) periods that will take up the nitrogen from the soil that could otherwise cause nitrate pollution of water.*
- *The establishment of fertilizer plans on a farm-by-farm basis and the keeping of records on fertilizer use.*
- *The prevention of water pollution from run-off and the downward water movement beyond the reach of crop roots in irrigation systems.*

Action Programmes should include measures to limit the land-application of all nitrogen-containing fertilizers. According to Annex III: "*The measures shall include rules relating to:*

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[2] "Vulnerable zones" are "all know areas of land in their territories which drains into waters affected by pollution and waters that could be affected by pollution", "whether groundwaters contain more than 50 mg/l nitrates or could contain more than 50 mg/l nitrates", "whether natural freshwater lakes, other freshwater bodies, estuaries, coastal waters and marine waters are found to be eutrophic or in the near future may become eutrophic".

- *Periods when the land application of certain types of fertilizer is prohibited.*
- *The capacity of storage vessels for livestock manure; this capacity must exceed that required for storage throughout the longest period during which land application in the vulnerable zone is prohibited, except where it can be demonstrated to the competent authority that any quantity of manure in excess of the actual storage capacity will be disposed of in a manner which will not cause harm to the environment.*
- *Limitation of the land application of fertilizers, consistent with good agricultural practice and taking into account the characteristics of the vulnerable zone concerned, in particular:*
  - *Soil conditions, soil type and slope.*
  - *Climatic conditions, rainfall and irrigation.*
  - *Land use and agricultural practices, including crop rotation systems; and to be based on a balance between: The foreseeable nitrogen requirements of the crops, and The nitrogen supply to the crops from the soil and from fertilization corresponding to:*
    - *The amount of nitrogen present in the soil at the moment when the crop starts to use it to a significant degree (outstanding amounts at the end of winter),*
    - *The supply of nitrogen through the net mineralization of the reserves of organic nitrogen in the soil,*
    - *Additions of nitrogen compounds from livestock manure,*
    - *Additions of nitrogen compounds from chemical and other fertilizers.*

These measures will ensure that, for each farm or livestock unit, the amount of livestock manure applied to the land each year, including by the animals themselves, shall not exceed a specified amount per hectare. The specified amount per hectare be the amount of manure containing 170 kg N. However: a) for the first four year action programme Member States may allow an amount of manure containing up to 210 kg N; b) during and after the first four-year action programme, Member States may fix different amounts from those referred to above. These amounts must be fixed so as not to prejudice the achievement of the objectives specified in Article 1 and must be justified on the basis of objectives criteria, for example:

- *Long growing seasons.*
- *Crops with high nitrogen uptake.*
- *High net precipitation in the vulnerable zone.*
- *Soils with exceptionally high denitrification capacity.*

EU Water Framework Directive

The EU Water Framework Directive (WFD) is a legislative framework that establishes the guidelines to protect and improve the quality of all water resources within the European Union (EC, 2000). These water resources include rivers, lakes, groundwater, transitional and coastal water up to one sea mile (and for the chemical status also territorial waters which may extend up to 12 sea miles) from the territorial baseline of a Member State.

Article 2 introduces the main definitions, including:

- *Groundwater* means all water, which is below the surface of the ground in the saturated zone and in direct contact with the ground or subsoil.
- *Aquifer* means a subsurface layer or layers of rock or other geological strata of sufficient porosity and permeability to allow either a significant flow of groundwater or the abstraction of significant quantities of groundwater.
- *Groundwater body* means a distinct volume of groundwater within an aquifer or aquifers.

The objectives of the Water Framework Directive (WFD) are laid down in Article 4. For groundwater, the WFD calls for:

- To implement measures to prevent or limit the input of pollutants into groundwater and to prevent the deterioration of the status of the groundwater body;
- To protect, enhance and restore all groundwater bodies, and ensure a balance between abstraction and recharge of groundwater, with the aim of achieving *good groundwater status*[3] by 2015.
- To reverse any significant and sustained upward trend in the concentration of any pollutant resulting from the impact of human activity in order to progressively reduce pollution of groundwater.

The WFD defines *good chemical status* as the status of a groundwater body such that:

- The concentrations of pollutants do not exhibit the effects of saline or other intrusions.
- Do not exceed the quality standards applicable under other relevant Community legislation and
- Are not such as would result in failure to achieve the environmental objectives specified under Article 4 for associated surface water nor any significant

[3] *Groundwater status* consists of two parts: quantitative status and chemical status and the overall status is taken to be the poorer of the two

diminution of the ecological or chemical quality of such bodies nor any significant damage to terrestrial ecosystems which depend directly on the groundwater body.

Good quantitative status is defined as:

- The level of groundwater is such that the available groundwater resource is not exceeded by the long-term annual rate of abstraction.
- Accordingly, the level of groundwater is not subjected to anthropogenic alterations such as would result in failure to achieve the environmental objectives specified under Article 4 for associated surface waters, any significant diminution in the status of such waters and any significant damage to terrestrial ecosystems which depend directly on the groundwater body.
- Alterations to flow direction resulting from level changes may occur temporarily, or continuously in a spatially limited area, but such reversals do not cause saltwater or other intrusions, and do not indicate a sustained and clearly identified anthropogenically induced trend in flow direction likely to result in such intrusions.

Article 7 requires the identification of all groundwater bodies used, or intended to be used, for the abstraction of more than 10 m^3 of drinking water a day as an average. By implication, this volume could be regarded as a significant quantity of groundwater.

To protect groundwater bodies and/or specific groundwater supplies against pollution it will often be necessary to constrain agricultural land-use practices in specific areas, as stated in article 7 named Waters used for the abstraction of drinking water, which says that the Member States shall protect all water bodies of water used for human consumption to avoid deterioration of their quality in order to reduce the level of purification treatment, it also mentions that the Member States may establish safeguard zones of those water bodies.

Another important aspect of the WFD is that, it is the first European Directive to explicitly recognize the importance of this interdependency between aquatic ecosystems and their socio-economic values and provides a much more integrated catchment approach to water policy (Brouwer et al., 2006).

The Directive clearly integrates economic aspects into water management and policy making. To meet the environmental objectives, the Directive calls for applying economic principles (e.g., the polluter pays principle), approaches (e.g., cost-effectiveness analysis), and instruments (e.g., water pricing). The economy has a decisive role in the development of river basin management plans and the design of water pricing policies. The WFD has assigned new roles to economics in water policy from financial studies to economic valuation (considering the economic value of water), at local to river basin scales, and to support project selection, strategies, and programs (Strosser 2004).

The key requirements concerning economics supporting the implementation of the WFD are (EC, 2003):

- Economic analysis of water use (such as forecast of water supply and demand, costs and prices of water services and investments needed and current level of cost recovery) (Article 5 and Annex III).
- Water price policies providing incentives for efficient and sustainable water use (Article 9).
- Ensuring an adequate contribution of the various water uses (such as industry, households and agriculture) to the recovery of water service costs based on the economic analysis and taking into account the polluter pays principle (Article 9).
- Implementation of the most cost effective combination of measures to achieve the good water status at each river basin by 2012 (Article 11).
- Justification of potential time and objective derogation when disproportionate costs are identified (Article 4).

The Guidance Document on the Economic Analysis (European Commission, 2003) advices that the various elements of the economic analysis should be integrated in the policy and management cycle in order to aid decision making when preparing the river basin plans. Additionally the Groundwater Summary Report (European Commission, 2005) was developed as a common strategy for supporting the implementation of the Water Framework Directive (2000/60/EC) establishing a framework for Community action in the field of water policy. The main aim of this strategy is to allow a coherent and harmonious implementation of the WFD.

<u>Groundwater Directive</u>

The Groundwater Directive (2006/118/EC) establishes specific measures in order to prevent and control groundwater pollution, including the pollution of nitrate from agricultural sources. These measures include in particular:

- Criteria for the assessment of good groundwater chemical status.
- Criteria for the identification and reversal of significant and sustained upward trends and for the definition of starting points for trend reversals.

Annex 1 of the Groundwater Directive states that the quality standard for nitrate (50 mg/l) applies to all groundwater bodies, with the exception of the Nitrate Vulnerable Zones identified under the Nitrate Directive. For each groundwater body, the degree to which it is at risk of failing to meet the objectives has to be assessed.

1.3 Thesis organization

The dissertation is organized into twelve chapters, including this introductory one and 4 appendixes. The second chapter presents a review of the state of the art on groundwater quality management and stochastic analysis of management schemes; some ideas on efficient allocation are also introduced in this chapter. Chapter 3 introduces to the process of nitrate groundwater pollution, from the nitrogen cycle at the soil to the nitrate transport and fate in groundwater. Chapter 4 presents the method for deriving the optimal fertilizer allocation and its application to an illustrative case study. In chapter 5 the methodology is applied to El Salobral-Los Llanos aquifer where optimal fertilizer applications were derived. The methodology was further extended to analyze the uncertainty in the conductivity field, which is presented in chapter 6. Finally the overall conclusions, limitations of the modeling approach and suggestions for future research to extend this approach are exposed.

2 Modeling policies for nitrate pollution abatement. State of the art.

This chapter starts with a brief introduction to the economics of nitrate pollution and the efficient allocation of pollution, followed by an overview of different methodologies and modeling efforts to assess the effect of agricultural policies and measures on groundwater nitrate pollution. Since a stochastic model is also developed for optimal management of fertilizers (design of fertilizer standards) to control groundwater nitrate pollution from agriculture under groundwater parameter uncertainty, the state-of-the-art on stochastic management models for groundwater pollution is also reviewed.

2.1 Economics and policies of nitrate pollution control

2.1.1 Introduction. Efficient allocation of pollution.

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.

2.1.2 Policies for agricultural pollution control

Different policies can be applied for controlling nitrate pollution from agricultural sources. One of them is the implementation of *agricultural best management practices* (BMPs). The BMP to minimize nitrate inputs to groundwater encompass a broad and diverse range of crop and soil management options as well as socio-economic and possibly regulatory activities (Keeny and Follet, 1991). The guiding principle is to minimize the amount of nitrate in the rooting zone, especially during periods when leaching is likely to occur. This could involve multiple fertilizer applications; use of cover crops or deep-rooted crops; genetic selection to improve crop *N*-use efficiency; chemical additives that inhibit the rate of nitrification; slow-release inorganic or organic fertilizers; carefully managed irrigation to minimize leaching; and inclusion of available *N* from NO_3 in the rooting zone and *N* mineralized from organic matter, manure, and crop residues in *N* fertilizer recommendations. Considerable refinement of *N*-fertilizer recommendations, taking into account such factors as weather, *N* cycling, and level of management, is needed. Other solutions may be required in extreme cases. These could include land-use zoning to lower the density of cropland in a watershed, a tax, or legal restrictions on fertilizer use. Crops often leave the land bare for a significant portion of the season. This offers the potential for nitrate leaching losses since crop uptake of *N* is not occurring for a major part of the year (Keeny and Follet, 1991). Excess NO_3 in the root zone must be avoided at times when soil is vulnerable to leaching by excess rainfall or irrigation.

Several economic and legal (mandatory) instruments have been suggested as a means of reducing nitrate contamination of ground and surface water. Taxes on nitrogen use, restrictions on the total quantity of nitrogen which can be applied, or restrictions on per-hectare nitrogen applications are included among the policy alternatives that have been proposed. Targeted policies have been suggested as alternative means of reducing the likelihood of nitrate losses in runoff and percolation. Targeted policies might focus on taxing or restricting nitrogen use on certain soils or restricting or taxing nitrogen use in certain production systems. Policies targeted to specific soils or productions systems would be difficult to monitor and may not have a significant impact on regional nitrate losses. However, targeted policies could reduce expected nitrate losses more per euro reduction in expected net returns than could broad policies. If these policies are implemented on a regional basis, each policy is likely to have a different impact on the expected quantity of nitrate lost in runoff and percolation, as well as on producer net returns. Tradeoffs between nitrate losses and net return reductions will likely vary by production situation and region (Mapp et al., 1994):

2.1.3 Economic analysis of agricultural nonpoint pollution.

There is a very extensive literature on the economics of nonpoint pollution, pioneered by the seminar papers by Griffin and Bromley (1982) and Shortle and Dunn (1986). Economic theory mentions different control mechanisms of agricultural non-point pollution externalities but these instruments cannot be readily implemented nor can their efficiency be promptly assessed (Shortle and Dunn, 1986). Policy mechanisms used for include direct regulations (i.e. standards on the amount and use of potential pollutants and production practices) and pricing policy like taxes or subsidies. Taxes and subsidies can be applied directly to the polluting emissions (‘‘effluent’’ taxes or subsidies) or based on some emission proxies like polluting inputs or certain agricultural practices (‘‘influent’’ taxes or subsidies). The paper by Segerson (1988) offered new perspectives in the design of economic instrument for controlling nonpoint pollution, analyzing the effectiveness of instruments based on measurements of ambient pollution instead of effluent or input instrument, given the difficulty to monitor individual pollution actions in practical terms. Much less studied are other economic incentives like tradable permits and contracts (Hahn, 2000).

Many studies have shown the potential role of water price policies in modifying farm-level irrigation decisions towards more environmentally friendly choices (Gardner and Young, 1988; Varela-Ortega et al., 1998; Berbel and Gomez-Limon, 2000). Some authors (Horan and Shortle, 2001) state that instruments based on irrigation water are more cost-efficient than instruments based on the use of nitrogen fertilization, while others (Martinez and Albiac, 2004; Semaan et al., 2007; Gardner and Young, 1988) have shown that water pricing is very inefficient to abate emissions.

Although the WFD only mentions water pricing, there are other economic instruments available as fertilizer taxes which have been widely studied, and many concluded that it is one of the best measures to reduce nitrates emissions (Martinez and Albiac, 2004; Semaan et al., 2007) while others say that taxes on applied nitrogen may increase nitrogen leaching (Haruvy, et al., 1997). Lally et al. (2007) compared regulation on nitrogen application versus taxes on fertilizer and concluded that a tax on inorganic nitrogen would impose a larger compliance cost on farmers and o public authorities than would a regulatory measure. Other researchers (Pan and Hodge, 1994, Johnson et al., 1991; Martinez and Albiac, 2004) claimed that taxing nitrogen emissions is the social optimum measure to reduce nitrate concentrations. Beside the economic efficiency of the different measures, the easiness of its application also should be taken into account. Segerson and Wu (2006) notes that mandatory regulations or restrictions and tax-based policies generally have "drawbacks in terms of inflexibility or high transaction or information cost". They suggest that the threat of the imposition of mandatory controls can be an effective mechanism for inducing firms to participate in voluntary agreements. In this context, a cost-minimizing voluntary agreement is considered as part of a subgame Nash equilibrium (Segerson and Wu, 2006).

Regarding the spatial scale of the analysis, many economic analyses of agriculture pollution have been conducted at the field of farm scale (e.g., Johnson et al., 1991; Knapp and Schwage, 2008), and just a few extended the analysis to the watershed scale (e.g. Gardner and Young, 1988; Mapp et al., 1994).

Other researchers have focused on assessing the economic cost of groundwater pollution by nitrates and pesticides. For example, Rinaudo et al. (2005) used the avoidance cost method combined with geostatistical methods for assessing scenarios of nitrate concentration evolution.

2.2 Modeling of nitrate abatement policies.

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, 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. They consider nitrate leaching as an indicator of groundwater pollution, therefore is not possible to determine if the policies analyzed can accomplish with required nitrate concentrations in groundwater. Moreover, the natural aquifer's ability to attenuate nitrate concentration is not taken into account, and the costs or policies obtained could result very conservative.

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 these cases, only the groundwater flow has been used to calculate the changes groundwater table so the pumping costs can be readjusted according to the different policies. But no transport models are used, therefore the attenuation of nitrate concentrations within the aquifer is not considered.

All the works mentioned above applied optimization in order to analyze the farmer's response and study the effects of different policies; however, as it was already mentioned, they do not consider nitrate transport in groundwater. Despite the considerable advances in the development of integrated tools for nitrate transport simulation at the catchment scale (e.g., Refsgaard et al., 1999; Lasserre et al., 1999; Birkinshaw and Ewen, 2000) these modeling 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, 2007; Graveline et al., 2007; Almasri and Kaluarachchi, 2007). This simulation approaches are useful for assessing "what if" scenarios, but do not provide optimal management solutions, since they are not integrated into an optimization framework.

Almasri and Kaluarachchi (2005), present a methodology for optimal nitrate management where a "black-box" statistical modeling approach (artificial neural networks) is used to relate on-ground nitrogen loadings with nitrate concentrations at specific control sites in a multi-criteria decision framework. The drawback of this methodology, is that using artificial neural networks the equations that define the physical problem are not included. Thus, if the physical conditions of the problem are changed, the validity of the solution can not be warranted.

2.3 Stochastic analysis of groundwater pollution: incorporating parameter uncertainty into decision making.

In order to improve groundwater quality it is necessary to analyze and implement management decisions, which increasingly relies on models. The modeling of nitrate contamination of groundwater in agricultural watersheds has mostly been addressed in a deterministic way; however, deterministic models can lead to failures in meeting the groundwater quality standards because of disregarding uncertainty.

The uncertainty comes from a wide variety of factors ranging from partial knowledge about the aquifer properties, its boundary conditions, land use practices, on-ground nitrogen loading, nitrogen soil dynamics, soil characteristics, depth to water table, flow and transport parameters affecting nitrate fate and transport in groundwater, to economic, regulatory and political factors. The effect of these uncertainties when managing groundwater resources for contaminated environments has been widely reported in the literature by using different approaches (Freeze and Gorelick, 1999).

A first approach is based on stochastic simulation-optimization methods. According to Wagner and Gorelick (1989), these stochastic optimization methods can be divided in two management model formulations. The first, termed the multiple realization or stacking management model, simultaneously solves the nonlinear simulation-optimization problem for a set of different scenarios representing uncertainty, e.g., by using a sampling of hydraulic conductivity realizations (Wagner and Gorelick, 1989; Aly and Peralta, 1999; Feyen and Gorelick, 2004; Feyen and Gorelick, 2005; Ko and Lee, 2009). This approach can provide reliable (over 90%) groundwater quality strategies based on a few number of scenarios as shown by Wagner and Gorelick (1989), which used a stack size of 30 conductivity realizations in a pump and treat remediation design.

The second model, termed the Monte Carlo management model, solves the nonlinear simulation-optimization problem individually for a single scenario representing uncertainty. Because they represent a simpler approach more works in the literature have pointed out towards this second model to assess the uncertainty (e.g., Gorelick 1983; Freeze and Gorelick 1999; Thorsen et al., 2001; Mayer et al. 2002; De Vries et al., 2003; Kroeze et al., 2003; Lacroix et al., 2005). This stochastic management approach has been combined with a stochastic algorithm to solve the coupled flow and mass transport inverse problem to design a reliable pump-and-treat scheme (Bakr et al., 2003). They used a nonlinear multiobjective formulation to explore the whole trade-off curve between reliability and cost of remediation. In the same line, Ko and Lee (2008) assessed the uncertainty by obtaining cumulative distribution functions (CDFs) of the remediation cost of a pump and treat method for different density and locations of hydraulic conductivity sampling in a contaminated zone.

A second approach is related to the probabilistic “chance-constrained” programming, which allow the determination of optimal groundwater quality management subject to a specified system performance reliability requirement (e.g., Tung, 1986; Wagner and Gorelick 1987; McSweeny and Shortle, 1990; Sawyer and Lin 1998; Wagner 1999). This approach has also the advantage of requiring less computational effort than the multiple realization model. In most of the works related to the chance-constrained technique, the obtained optimal design satisfies the stochastic constraints with a predetermined probability distribution, which represents the uncertainty of aquifer parameters. For mathematical convenience, the most widely used statistical model is the normal distribution (e.g., Tung, 1986). However, it is possible to use stochastic constraints with a distribution-free approximation (e.g., Fuessle, et al., 1987).

A third approach was presented by Morgan et al. (1993), which combined the advantages of the simulation-optimization models with those of the chance-constrained models. Again, the designer can select the degree of reliability, which is accomplished by allowing a certain number of the Monte Carlo realizations to fail. Moreover, this technique considers uncertainty in all linear programming constraint coefficients and does not require a priori knowledge of the distribution. Other authors have applied this technique, called mixed-integer-chance-constrained programming (MICCP), e.g., Ritzel et al. (1994) and Dhar and Datta (2007).

However, most of the works belonging to the three different approaches above mentioned refer to pump and treat methods for obtaining the optimal remediation strategy of contaminated aquifers, i.e., the locations and rates of extraction wells and/or the required remediation time are optimized. Some articles also deal with the design of monitoring networks for detection of groundwater pollution (Dhar and Datta, 2007). Most paper on non-point nitrogen pollution under uncertainty consider uncertainty with regard to the hydraulic conductivity or regional boundary conditions (e.g., Wagner and Gorelick, 1989; Feyen and Gorelick, 2004), although some of them consider other sources of uncertainty. For instance, Van den Brink et al. (2008) assessed the uncertainty of the calculated concentrations of nitrate leached into groundwater for the various combinations of land use, soil type, and depth of the groundwater table by means of a Monte Carlo simulation technique in combination with a Latin hypercube sampling procedure, being all embedded in a negotiation support system (NSS). Some of these contributions make use of a ‘‘black-box” statistical modeling approach (artificial neural networks or genetic algorithms) to relate on-ground nitrogen loadings with nitrate concentrations at specific control sites in a multicriteria decision framework (e.g., Aly and Peralta, 1999; Ritzel et al., 1994).

3 Groundwater nitrate pollution. Bio-physico-chemical processes.

Nitrate groundwater contamination results from several processes from pollution sources to water bodies, including nitrogen leaching and pollution reactions, fate and transport. Once nitrogen enters the soil, it undergoes several biochemical transformations before leaching to groundwater mostly as nitrate. 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.

3.1 Nitrogen cycle

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).

Organic nitrogen consists of compounds from amino acids, amines, proteins and humic compounds with low nitrogen content. Inorganic nitrogen consists of ammonium, nitrite and nitrate forms. Nitrogen form untreated or partially treated wastewater discharges or human waste fertilizers may be in either organic or ammonium form, while nitrogen from chemical fertilizers will typically be in ammonium or nitrate form.

The mayor sources of nitrates in groundwater include intensive animal operations, irrigated and row crop agriculture, septic tanks and other sources as landfills can be of concern in localized areas. The organic nitrogen is originated from the organic matter from plants and animals. Another sources of nitrogen is atmospheric, that trough fixation it can be incorporated into a chemical compound such that it can be used by plants and animals, Figure 3.1 Fixation of nitrogen form N_2 gas to organic nitrogen is predominantly accomplished by specialized microorganisms and the associations between such organisms and plants (Canter, 1996).

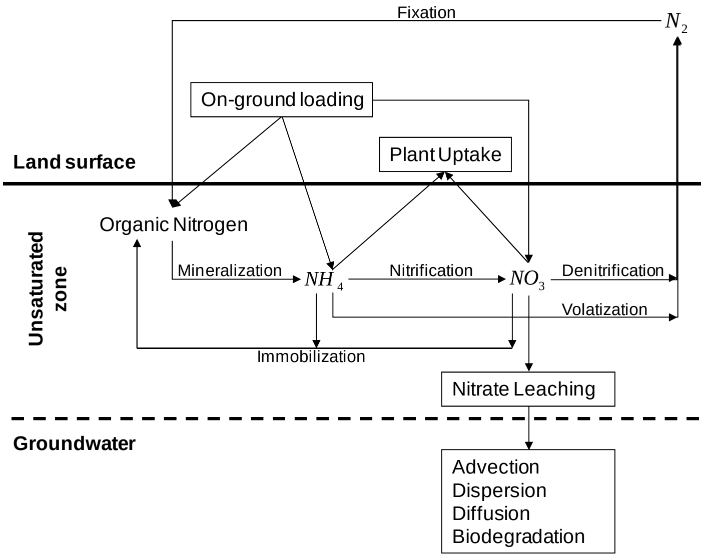

Figure 3.1 Nitrogen cycle

The organic nitrogen can undergo a transformation called mineralization or ammonification which refers to the biological decomposition of organic materials in soils and their conversion to inorganic forms (NH_4 and NO_3), the process requires an energy source for the soil microorganisms such as crop residues and other organic matter materials, a favorable temperature, and suitable soil moisture conditions (Schepers and Moiser, 1991). Then this ammonium can undergo nitrification. Nitrification refers to the biological oxidation of ammonium ions NH_4, this is accomplished in two steps: first to the nitrite form NO_2, then to the nitrate form NO_3; two specific chemoautotrophic bacteria are involved, the Nitrosomonas and the Nitrobacter. The transformation reactions are generally coupled and proceed rapidly to the nitrate form; nitrite levels at any given time are relatively low. The nitrate formed can be used in synthesis to promote plant growth, or it can be subsequently reduced by denitrification (Canter, 1996).

Denitrification is the biological reduction of nitrate to nitrogen gas N_2, the reduction can proceed through several steps in a biochemical pathway. A fairly broad range of heterotrophic bacteria are involved in the process, requiring an organic carbon source of energy. For denitrification to proceed, anoxic conditions must usually exist, although this is not strictly the case for all bacteria.

Immobilization is the biological conversion of NO_3 or NH_4 into microbial tissue, thus making the N unavailable for immediate utilization by the crops (Schepers and Moiser, 1991).

Losses of *N* through the **gaseous emissions** may occur either directly from the plant or from the soil. Losses of *N* are principally as ammonia (NH_3) from maturing plant vegetation, such volatile *N* losses occur after plant flowering and have been found in a variety of crops.

Losses of fertilizer and soil *N* from the plant root zone are known to occur as a result of soil microbial reactions as well as direct NH_3 volatilization. Although denitrification is considered to be the single most important *N* loss mechanism, sufficient data area available only to show that the amount of *N* lost can be quite variable and that if saturated soil moisture conditions can be avoided during the time that soil NO_3 concentrations are high then *N* loss by denitrification can be minimized. *N* losses by denitrification are related to soil organic matter content and drainage class (Schepers and Moiser, 1991).

Additions of *N* to a crop, other than through fertilization, come from the atmosphere. The mechanism of additions that are identified include *N* dissolved in precipitation, dry deposition, and direct plant absorption of gaseous ammonia.

Leaching is generally a major pathway of *N* loss in humid region agriculture and under irrigation; estimates commonly range between 5 and 50% of the *N* inputs (Maisinger et al., 1991). Small losses are likely if *N* inputs do not exceed the crop assimilation capacity, if the *N* is applied in phase with crop demand, and if soil NO_3-N concentrations are low when drainage is occurring.

To produce a quantitative prediction of NO_3 leaching it is require detailed hydrologic models and detailed *N* transformation models.

More than 90% of the nitrogen present in soil is organic, either in living plants and animals or in humus originating from 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 soil 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 properly understand and simulate the interaction of the aforementioned factors in order to account for the transient and spatially variable nitrate leaching to groundwater.

3.2 Agriculture as a source of groundwater pollution

Nitrogen is an essential nutrient to plants and it is often a limitation to the growth of plants. However, applying more nitrogen than is needed for the optimum crop yield greatly increases nitrate losses by leaching. The application of nitrogen fertilizer in agriculture has been very cost-effective; the extra value of the crops produced has out-weighted the cost of applying it. This has motivated the farmers to apply plenty of fertilizer to ensure the maximum yield which creates a surplus of inputs over outputs in the crop (Hatch et al., 2002).

For arable farming, the weather dominates N loss through the impact of rainfall and temperature on drainage, crop growth and N utilization. Besides the weather, losses from agricultural lands are determined by (Hatch et al., 2002): residual mineral N concentrations present in the soil, cultivation, drilling date, amount and timing of N fertilizer and manures applied, legume rotation, etc.

3.2.1 Soil-crop system

Whole crop systems place the lower bound just below the crop root zone and thus include the standing crop plus its roots. These systems require root residues estimates, soil N transformations within the system and have a steady state condition. Nitrogen budgets are based on the concept of mass conservation. Maisinger and Randall (1991) defined the Long Term Potentially Leachable total *N* (LPLN) as the difference between total *N* inputs and total *N* outputs (excluding *N* leaching) minus the change in *N* storage term ΔN_{st} :

$$LPLN = N_{inputs} - N_{outputs} - \Delta N_{st} \tag{3.1}$$

This equation gives us the potential *N* leachable, it is the calculated excess total *N* which could leach from the system during drainage events and thus potentially affect groundwater quality. In dry areas *LPLN* may not reach groundwater in years or even in decades, depending on the hydrologic conditions. This equation is a simplification since only NO_3-*N* is mobile in soils and organic *N* is immobile. However, if viewed over the long term the organic *N* component can certainly be subject to potential leaching as it mineralizes over time. The impact of *LPLN* on groundwater quality may also be affected by *N* transformations in the vadose zone.

The interpretation of the *LPLN* should rest on the fact it is the long term average excess *N* input above the estimated *N* output, with regard to the likely change in *N* stored within the system. This excess *N* may or may not leach from the system depending on the hydrologic conditions.

Nitrogen inputs

The largest agricultural *N* cycle inputs are usually fertilizer *N*, manure *N*, symbiotically fixed *N*, and irrigation water *N*. Secondary *N* inputs are the *N* received in precipitation, dry deposition of *N* (ammonia absorption), crop seed, and non-symbiotic N_2 (Maisinger and Randall, 1991).

Nitrogen outputs

The largest agricultural *N* cycle outputs (excluding leaching) are *N* removed in harvested crops, denitrification and ammonia volatilization. Secondary *N* outputs include soil erosion, surface runoff losses, miscellaneous gaseous *N* losses, and gaseous *N* losses from maturing crops (Maisinger and Randall, 1991).

Change in nitrogen storage

The change in the storage term ΔN_{st} is the difference in total *N* content at the end of the time step less the total *N* at the beginning. This term is made up of an inorganic *N* component which is the change in soil NO_3-*N*, and an organic *N* component which is the change in soil organic *N* over time.

The soil NO_3-*N* content is much smaller than the soil organic N content, but it is an active entity because NO_3-*N* is readily taken up by plants, is soluble and mobile in soils, and is lost through denitrification. The change is soil organic *N* is a difficult quantity to estimate because the soli organic *N* pool is large and only slowly reactive, long time steps will be required to measure changes in this pool, 3 to 10 years depending on the climate and cultural practices (Maisinger and Randall, 1991).

Crop nitrogen requirements

Nitrogen fertilizer is known to increase yield of many crops. Yield response to *N* fertilizer vary depending on the amount of inherent plant-available *N* in the soil at the beginning of the growing season (residual soil *N*), and *N* supplied throughout the season by organic matter decomposition (mineralization) and *N* in precipitation and irrigation water. Maximum yields are unique for a given crop variety as it interacts with local growing conditions such as climate, soils, nutrient supply, and competition by various pests (Schepers and Moiser, 1991).

Crop *N* requirement will be determined by yields that are economically profitable (incremental increase in crop value divided by incremental cost of *N* fertilizer is greater than 1), although these may not be the maximum attainable yields.

In fertilizer management, a balance between food production, profit and environmental quality must be maintained. Improved *N*-use efficiency can reduce in-season *N* losses or produce lower amounts of residual nitrate following the cropping season. These improvements can ultimately reduce the amount of *N* that leaches to groundwater. Over time *N* applied often as exceeded that removed in the crops, resulting in higher residual nitrate levels in soil and, in some cases, higher nitrate levels in groundwater (Bock and Hergert, 1991).

The relationship of yield with increasing *N* rate is usually curvilinear, at higher rates yield increase per unit of *N* decreases until no further yield increase is attained. Adding *N* beyond that required for maximum yield has little adverse effect on grain yield, but often decreases the yield of some crops.

Application of *N* just before the time of most rapid *N* uptake assures the best crop use of *N*. Much of the leaching potential exists between cropping seasons or before crops starts growing rapidly. In these situations, post-plant application of *N* is effective because of the timing of *N* supply in relationship to crop *N* uptake. Adding a nitrification inhibitor with pre-plant *N* delays conversions of ammonium to nitrate and can also reduce the possibility of nitrate leaching. In irrigated areas, applying *N* with irrigation water just preceding maximum *N* uptake periods is another good method for improving *N*-use efficiency (Bock and Hergert, 1991).

3.2.2 Water and nitrogen percolation

The amount of water that percolates through and below a crop's root zone is very important in determining the amount of nitrate leached to groundwater. The amount of water that percolates from soil is determined in part by the balance between gains in soil water by rainfall or irrigation and losses from the soil water storage reservoir from crop water use and evapotranspiration.

Water stored in the soil varies greatly in the amount of energy required to remove it from the soil. Gravitational force causes water to percolate from the soil when the water content is between saturation and field capacity. As the soil water content falls below field capacity because the crop use and evaporation, the remaining water is held more tightly by the soil. Water removal by crops can continue until the water level reaches the wilting point. At this level, water is attracted so strongly to soil that plant root removal of water nearly ceases.

Percolation and nitrate losses are usually more severe when a crop is not present in the filed (Williams and Kissel, 1991). However, on very sandy soils, substantial percolation early in the cropping season can still occur, depending on the timing of rainfall events. There will generally be less percolation from single rainfall events when a crop is growing compared to the situation without crop. Therefore, given equal rainfall, geographical locations that receive peak rainfall during the cropping season should have less percolation than locations that have peak rainfall at times when no crop is growing or the crop is immature.

Several soil characteristics in combination with weather and crop factors control the transformations of *N* and the movement of water in the soil. These processes control the potential for leaching NO_3 out of the rooting zone to an aquifer. Soil permeability, water storage capacity, texture and thickness strongly influence the amount of water that percolates through the soil and the length of time that biological and chemical processes have to alter *N* loads in the root zone (Knox and Moody, 1991).

Ammonium-nitrogen may not be transported through the **u**nsaturated zone and into the groundwater due to adsorption, cation exchange, incorporation into microbial mass or release to the atmosphere in the gaseous form. Adsorption is probably the major mechanism of removal in the subsurface environment. Under anaerobic conditions in the subsurface environment, positively charged ammonium ions NH_4 are readily adsorbed onto negatively charged soil particles. Since anaerobic conditions in soils are usually associated with saturated soils, some movement of ammonia with groundwater can occur.

3.3 Nitrogen movement in groundwater

Nitrate is typically more mobile in the subsurface environment than ammonium nitrogen. 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.

The flow of fluids through porous media is governed by the laws of physics, since the flow is a function of several variables. It is usually described by partial differential equations in which the spatial coordinates x, y and z and time t are the independent variables.

In deriving the equations, the laws of mass and energy conservation are employed. The law of conservation or continuity principle, states that there can be no net change in the mass of a fluid contained in a small volume of an aquifer. Any change in mass flowing into the small volume of the aquifer must be balanced by a corresponding change in mass flux out of the volume, or a change in the mass stored in the volume, or both. The law of conservation of energy states that within any closed system there is a constant amount of energy, which can be neither lost nor increased; it can, however, change form (Fetter, 2000). Darcy's law states that the rate of water flow through a porous media is proportional to the difference in the height of the water between the two ends of the porous filter and inversely proportional to the length of the flow path. Derived upon these principles the main equation of groundwater movement can be derived.

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):

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

(3.2)

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).

There are three transport mechanisms: advection, molecular diffusion and mechanical dispersion. The advective transport is the process where dissolved solids are carried along with the flowing groundwater. The amount of solute that is being transported is a function of its concentration and the quantity of the groundwater flowing. A solute in water will move from an area of greater concentration towards an area where it is less concentrated. This process is known as molecular diffusion. Diffusion will occur as long as concentration gradient exists, even if the fluid is not moving. In porous media, diffusion cannot proceed as fast as it can in water because the ions must follow longer pathways as they travel trough the soil pores. To account for this, an effective diffusion coefficient is used.

Groundwater moves at rates that are both greater and less than the average flow velocity. At macroscopic scale there are three basic causes of this phenomenon (Fetter, 1998):

- as fluid moves through the pores, it will move faster in the center of the pore that along the edges,
- some of the fluid particles will travel along longer paths in the porous media than other particles to go the same linear distance and
- some pores are larger than others which allows the fluid flowing through these pores to move faster. Because the invading solute-containing water is not all traveling at the same velocity, mixing occurs along the flowpath, this mixing is called mechanical dispersion, and it results in a dilution of the solute at the advancing edge of the flow.

If we assume that mechanical dispersion can be described by Fick's law for diffusion and that the amount of mechanical dispersion is a function of the average linear velocity, then we can introduce a coefficient of mechanical dispersion. This is equal to a property of the medium called dynamic dispersivity, α, times the average linear velocity.

The process of molecular diffusion cannot be separated from mechanical dispersion in flowing groundwater. Therefore the two are combined to define a parameter called the hydrodynamic dispersion coefficient.

The advection-dispersion equation can be derived based on the conservation of mass of solute flux into and out of a small representative elementary volume of the porous media, the solute storage and the three transport mechanisms explained above.

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):

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

(3.3)

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.

4 Hydroeconomic modeling framework

The objective of the analysis conducted herein is to find the most cost-effective allocation for the reduction of fertilizer application in order to meet groundwater quality objectives. In other words, which area has to reduce emissions and by how much to be able to achieve the policy objectives at the least cost.

This work also deals with the optimal scheduling of periodic controllable sources of groundwater pollution in such a way that water quality at selected locations is protected and the profit reduction in the agricultural activities is minimized.

This chapter presents the methodology developed, which is then applied to both a synthetic and a real case study, the Salobral-Los Llanos aquifer in the Mancha Oriental groundwater body (chapter 5).

4.1 Deterministic 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.

In the proposed hydro-economic modeling 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:

$$Max\, \Pi = \sum_{s} \sum_{y} \frac{1}{(1+r)^{y}} A_{s} \left(p_{s} \cdot Y_{s,y} - p_{n} \cdot N_{s,y} - p_{w} \cdot W_{s,y} - C_{s} + S_{s} \right) \tag{4.1}$$

subject to:

$$\sum_{s} RM_{c\times t, s\times y} \cdot cr_{s\times y} \leq q_{c\times t} \quad \forall c,t,y \tag{4.2}$$

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_s is the area cultivated for crop located at source *s*; p_s is the crop price (€/kg); $Y_{s,y}$ is the production yield of crop located at source *s* at planning year *y* (kg/ha), that depends on the nitrogen fertilizer and irrigation water applied; p_n is the nitrogen price (€/kg); $N_{s,y}$ is the fertilizer applied to crop located at source *s* at year *y* (kg/ha), p_w is the price of water (€/m^3), and $W_{s,y}$ is the water applied to crop located at source *s* at each planning year *y* (m^3); C_s is the aggregation of the remaining per hectare costs for crop located at source *s* (€/ha); S_s are the subsidies for the crop located at source s (€/ha); *r* is the annual discount rate, *RM* is the unitary pollutant concentration response matrix where each column is the nitrate concentration for each crop area *s* times de number of years within the planning horizon *y*, the number of rows equals the number of control sites *c* times the number of simulated time steps *t* in the frame of the problem; *q* is a vector of water quality standard imposed at the control sites over the simulation time (kg/m^3); *cr* is a vector made up of three components, which corresponds to the nitrate concentration recharge (kg/m^3) reaching groundwater from a crop located at source s, whose components are given by:

$$cr_{s\times y} = \frac{L_{s\times y}}{r_{s\times y}} \tag{4.3}$$

where r_{sxy} is the water that recharges the aquifer at source s (m^3/ha) at planning period y; and L_{sxy} is the nitrogen leached from each crop area (kg/ha). The sub-index y 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 (Figure 4.1).

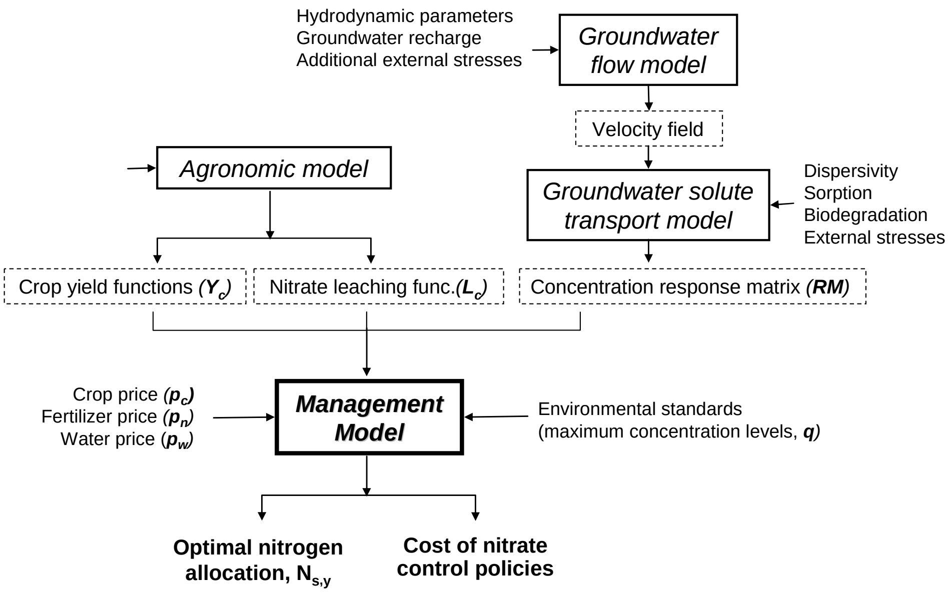

Figure 4.1 Flowchart describing the modeling framework

Groundwater flow and transport governing equations are represented within the management model through the pollutant concentration response matrix *[RM].*

4.1.1 Pollutant Response Matrix Method

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, 1974). 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 Daily, 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 transient flow.

The response matrix describes the influence of pollutant sources upon concentrations at the control sites over time. The simulation model was used to develop unit source solutions which are assembled to form the concentration response matrix.

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 (Figure 4.2).

Sources *x* Planning horizons (sxy)

Control sites *x* Time (cxt)

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

Figure 4.2 Response matrix configuration

The quality restriction can be different for each control site and can change over time. 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. Numerical simulation models based on the flow and solute transport governing equations were used to develop the pollutant concentration response matrix. MODFLOW (McDonald and Hargough, 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).

4.1.2 Agronomic simulation

Agronomic models are used to simulate plant growth and its yield under different conditions. One result of these kinds of models is the crop production functions for certain conditions. There are several agronomic models. In this work we used the results of the

EPIC[4] package (Williams, 1995). This software simulates crop growth using local conditions on soil, climate, irrigation water, tillage and other operations. By means of this package, the production and pollution functions can be estimated. The crop yield, required to estimate the crop benefits was calculated through production function according to the following polynomial equation, calibrated with the values simulated with the EPIC package:

$$Y_{s,y} = a + b \cdot W_{s,y} + c \cdot W_{s,y}^2 + d \cdot N_{s,y} + e \cdot N_{s,y}^2 + f \cdot W_{s,y} \cdot N_{s,y} \tag{4.4}$$

where $Y_{s,y}$ is the crop yield located at source s for a year y (kg/ha), $W_{s,y}$ is the water applied to the crop located at source s (m^3/ha) and $N_{s,y}$ is the fertilizer applied to the crop located at source s (kg/ha) within the year y. The coefficients a,…,f are calibrated (for example by a least-square fitting technique) with the values simulated with the EPIC package.

The amount of leaching and hence the amount of nitrates in groundwater have been found to be a function of the timing of fertilizer application, vegetative cover, soil porosity, fertilizer application method, irrigation rate (Canter, 1996). Once the nitrogen is applied to the crop it suffers some transformation as explained in Chapter 3. After the plant uptake and the transformation, some of that nitrogen applied is converted into nitrate that can leach to the aquifer. The amount of nitrogen leached was introduced into the management model as quadratic functions as follows:

$$L_{s,y} = g + h \cdot W_{s,y} + i \cdot W_{s,y}^2 + j \cdot N_{s,y} + k \cdot N_{s,y}^2 + l \cdot W_{s,y} \cdot N_{s,y} \tag{4.5}$$

where $L_{s,y}$ is the nitrogen leached (kg/ha), $W_{s,y}$ is the water applied to the crop located ar source s (m^3/ha) with in the year y, and $N_{s,y}$ is the fertilizer applied to the crop located at source s (kg/ha). The coefficients g,…,l are calibrated (for example by a least-square fitting technique) with the values simulated with the EPIC package.

The nitrate leached in (kg/ha) is diluted by the irrigation water recharge, therefore the nitrate concentration $cr_{s,y}$ entering the aquifer is:

$$cr_{s \times y} = \frac{L_{s \times y}}{r_{s \times y}} \tag{4.6}$$

[4] Environmental Policy Integrated Climate model developed by the USDA

where r_{sxy} is the water that recharges the aquifer (m^3/ha) at planning period *y*, and L_{sxy} is the nitrogen leached from each crop area *s* (kg/ha) at planning period *y*. The sub-index *y* in the formulation refers to the year within the planning horizon or the number of successive years in which the fertilizer is applied. The vector of n elements cr_{sxy} correspond to concentration recharge (the product of the concentrations of the source waters times the volumetric water fluxes), during the management period *y* and the disposal site location *s*.

This analysis assumes profit-maximizing firms; this means that, in absence of nutrient abatement policies, the firms will choose those levels of production and emissions that maximize their net profits. Each measure to decrease nutrient emissions then reduces profits. Situations in which some sectors reduce nutrient emissions to allow others to increase their emissions, while still achieving the overall reduction target, can only exist if increasing nutrient emissions is beneficial to the sectors concerned. The optimal solution of the management problem corresponds to a Pareto optimal condition, in which no firms can increase their profits with the same nutrient abatement requirement without a reduction in the profits corresponding to other crop areas. Whenever farmers (and other polluters as sewage treatment plants) are free to choose measures to reduce nutrient emissions, they are assumed to start with the cheapest options and to apply the more expensive options only if nutrient abatement requirements become tighter

GEPIC

GEPIC is a GIS-based crop growth model integrating a bio-physical EPIC model (Williams et al., 1989; Williams, 1995) with a GIS to simulate the spatial and temporal dynamics of the mayor processes of the soil-crop-atmosphere-management systems (Liu et al., 2009). The GEPIC model treats each grid cell as a site. It simulates the crop related processes for each predefined grid cell with spatially distributed inputs.

EPIC

EPIC model (Williams et al., 1989; Williams, 1995) is a continuous simulation model that can be used to determine the effect of management strategies on agricultural production and soil and water resources. The major components in EPIC are weather simulation, hydrology, erosion-sedimentation, nutrient cycling, pesticide fate, plant growth, soil temperature, tillage, economics, and plant environment control.

The model is processes based and runs on a daily steps, the main input data required is daily weather data, soil properties, crop-specific growth parameters and farm management practices.

Crop growth

Crop growth is simulated by modeling leaf area, light interception and converting it into biomass. The leaf area index depends upon heat units, maximum leaf area index, a crop parameter that initiates leaf area index decline, and stress factors. Interception of solar radiation is estimated as a function of the crop's leaf area index.

Plant growth is constrained by water, nutrient, and temperature stresses. The potential biomass is adjusted daily if one of the plant stress factors is less then 1.0. The water stress factor is computed by considering supply and demand. The temperature stress factor is estimated using a function dependent on the daily average temperature, the optimal temperature, and the base temperature for the crop. The N and P stress factors are based on the ratio of accumulated plant N and P to the optimal values. The aeration stress factor is estimated as a function of soil water relative to porosity in the root zone (Williams, 1995).

The crop yield is estimated using the harvest index which increases as a nonlinear function of heat units from zero at the planting stage to the optimal value at maturity, using the following equation:

$$YLD = HIA \cdot B_{AG} \tag{4.1}$$

where YLD is the amount of economic dry yield could be removed from the field in kg/ha, HIA is the water stress adjusted harvest index (Liu, 2009). B_{AG} is the above-ground biomass on the day of harvest and is calculated as the sum of the daily actual increase in biomass in growing season:

$$B_{AG} = \sum_{i=1}^{N} \Delta B_{a,i} \tag{4.2}$$

The harvest index may be reduced by high temperature, low solar radiation, or water stress during critical crop stages. The harvest index is reduced by water stress using the following equation:

$$HIA_i = HIA_{i-1} - HI\left(1 - \frac{1}{1 + WSYE \cdot FHU\left(0.9 - WS_i\right)}\right) \tag{4.3}$$

where *HI* is the potential harvest index on the day of harvest, *WSYF* is a crop parameter expressing the sensitivity of harvest index drought, *FHU* is a crop growth stage factor, and *WS* is the water stress factor, and subscript *i* and *i-1* are the Julian days of the year.

Nitrate leaching

EPIC considerers as nitrate losses the leaching, surface runoff and lateral subsurface flow. The transformations in the soil consists of denitrification, mineralization, immobilization, nitrification and volatilization it also considerers as an input the N contribution from rainfall (Figure 4.3).

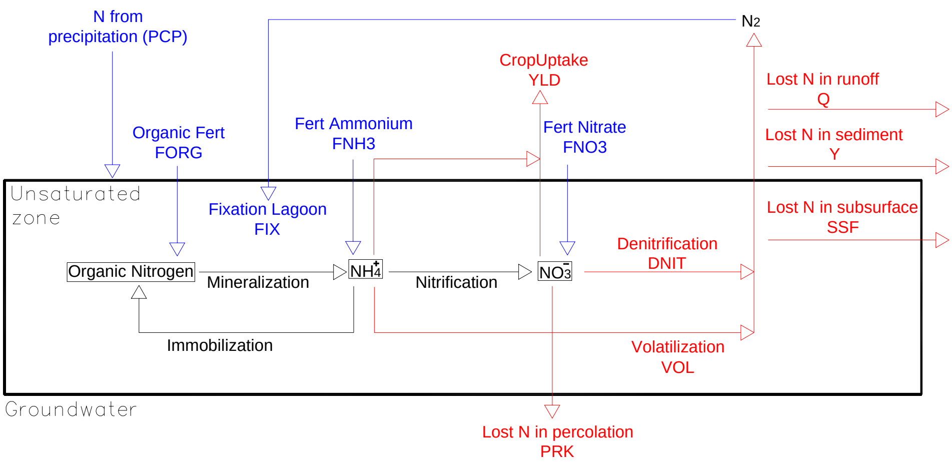

Figure 4.3 Processes taken into account in EPIC

Denitrification is a function of temperature and water content. The equation used to estimate the denitrification rate is (Williams, 1995):

$$DN_l = WNO3_l\left[1-\exp\left(-1.4\left(TF_{Nl}\cdot C_l\right)\right)\right], \quad SWF \geq 0.95$$

$$DN = 0\,, \qquad\qquad SWF \leq 0.95$$

(4.4)

where: *DN* is the denitrification rate in layer *l* in kg·ha^{-1}·d^{-1}, TF_N is the nutrient cycling temperature factor, *C* is the organic carbon content in %, *WNO3* is the weight of NO_3 and *SWF* is the soil water factor[5].

The model considers two sources of mineralization: fresh organic *N* pool, associated with crop residue and microbial biomass, and the stable organic *N* pool associated with the soil humus. Mineralization from the fresh organic *N* pool is estimated with the equation:

$$RMN_l = (DCR_l)(FON_l) \tag{4.5}$$

where: *RMN* is the *N* mineralization rate in kg·ha^{-1}·d^{-1} for fresh organic *N* in layer *l*, *DCR* is the decay rate constant for the fresh organic *N*, and *FON* is the amount of fresh organic *N* present in kg/ha. The decay rate constant is a function of C:N ratio, C:P ratio, composition of crop residue, temperature, and soil water.

The daily amount of immobilization is computed by subtracting the amount of N contained in the crop residue from the amount assimilated by the microorganisms:

$$WIM_l = (DCR_l)(FR_l)(0.0016 - C_{NFR}) \tag{4.6}$$

where: *WIM* is the *N* immobilization rate in layer l in kg·ha^{-1}·d^{-1}; 0.016 is the result of assuming that *C=0.4 FR*, that C:N of the microbial biomass and their labile products = 10, and that 0.4 of *C* in the residue is assimilated; and C_{NFR} is the *N* concentration in the crop residue in g/g, *FR* is the crop reidue. Immobilization may be limited by N or P availability.

The nitrification is estimated using the first-order kinetic rate equation:

$$RBV_l = WNH3_l\left(1 - \exp\left(-AKN_l - AKV_l\right)\right) \tag{4.7}$$

where: *RNV* is the combined nitrification and volatilization kg·ha^{-1}·d^{-1}, *WNH3* is the weight of NH_3 in kg/ha, *AKN* is the nitrification regulator, and *AKV* is the volatilization regulator for soil layer *l*. The nitrification regulator is a function of temperature, soil water content, and soil pH.

Volatilization of surface-applied ammonia is estimated as a function of temperature and wind speed, using the equation (Williams, 1995):

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[5] Soil Water Factor is the relation between soil water content and field capacity.

$$AKV_l = (TF_l)(WNF)$$

(4.8)

where: *AKV* is the volatilization regulator and *WNF* is the wind speed factor for surface application (soil layer 1) and *TF* is a temperature factor.

Depth of ammonia within the soil, cation exchange capacity of the soil, and soil temperature are used in estimating below surface volatilization.

Nitrate leaching is simulated by using an exponential function to describe the decrease in nitrate concentration caused by water flowing through a soil layer. The amount of NO_3-N lost when water flows through a layer is estimated by considering the change in concentration (Williams, 1995):

$$VNO3 = QT \cdot C_{NO3}$$

(4.9)

where: *VNO3* is the amount of NO_3-N lost from a soil layer and C_{NO3} is the average concentration of NO_3-N in the layer during percolation of volume *QT* through layer. At the end of the day, the amount of NO_3-N left in the layer is:

$$WNO3 = WNO3_0 - QT \cdot C_{NO3}$$

(4.10)

where: $WNO3_0$ and *WNO3* are the weights of NO_3-N contained in the layer at the beginning and ending of the day. The NO_3-N concentration can be calculated by dividing the weight of NO_3-N by the water storage volume:

$$C'_{NO3} = C_{NO3} - C_{NO3}\left(\frac{QT}{bl \cdot PO}\right)$$

(4.11)

where: C'_{NO3} is the concentration of NO_3-N at the end of the day, *PO* is soil porosity, and *bl* is a fraction of the storage *PO* occupied by percolating water.

The average concentration during the percolation of *QT*:

$$C_{NO3} = \frac{VNO3}{QT}$$

(4.12)

Amounts of NO_3-N contained in runoff, lateral flow and percolation are estimated as products of the volume of water and the concentration from the above equation.

4.2 Illustrative example. Synthetic case study application

4.2.1 Case study description

The modeling framework was applied to a hypothetical groundwater system. The system in Figure 4.4 is an aquifer with lateral impermeable boundaries and a steady flow directed from top to bottom of the figure. The finite difference grid is 30x41 km with a grid size of 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 a longitudinal dispersivity of 10 meters and a transversal dispersivity of 1 meter. The natural recharge is 500 m^3/ha. There are 70 stress period of one year (365 days) each one. Seven crop zones with five different crops are considered. For each crop a quadratic production function and a leaching function have been defined. There are 3 control sites in which nitrate concentration must not exceed 50 mg/l. Each source is related to a crop as shown in Figure 4.4.

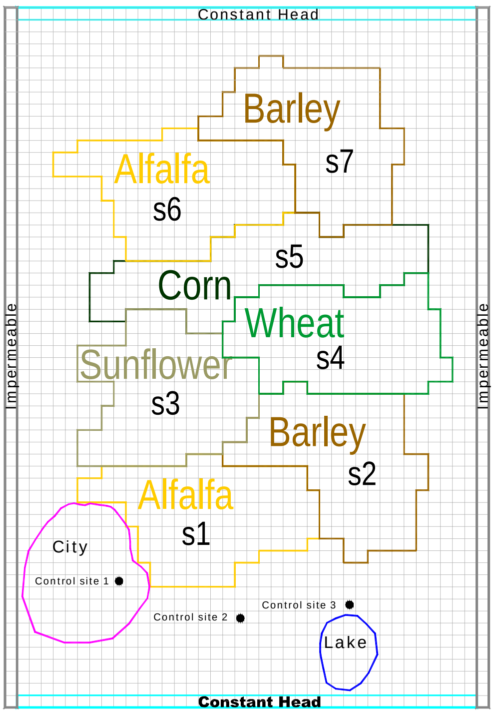


Figure 4.4 Groundwater system configuration

The production and nitrate leaching functions used are the ones showed in chapter 5 with the coefficients shown in Table 4.1.

Table 4.1 Production and leaching functions coefficients

Production functions coefficients						
Crop	**a**	**b**	**c**	**d**	**e**	**f**
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
Leaching functions coefficients						
Crop	**g**	**h**	**i**	**j**	**k**	**l**
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

For the management model the irrigation water was kept constant at the level where the yield is maximum. The irrigation water used is shown in Table 4.2. This table also shows the crop price considered in the management model. The nitrogen fertilizer price is assumed to be 0.60 €/kg. The area for each source is 3,600 ha. For this example neither fix costs nor subsidies were considered.

Table 4.2 Sources, crops and irrigation

Source	Crop	Area (ha)	Water applied (mm)	Crop price (€/kg)
S1	Alfalfa	3,600	950	0.09
S2	Barley	3,600	300	0.12
S3	Sunflower	3,600	400	0.30
S4	Wheat	3,600	250	0.13
S5	Corn	3,600	700	0.12

4.2.2 Pollutant concentration response matrix and breakthrough curves

Simulating unit nitrate leaching rate into groundwater the breakthrough curves for the different pollution sources were generated solving the flow equation with MODFLOW (McDonald and Harbough, 1988) a three dimensional finite difference groundwater flow model, and the solute transport with MT3DMS (Zheng and Wang, 1999) a modular three dimensional multi-species transport model for simulation of advection, dispersion, and chemical reactions of contaminants in groundwater systems.

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 and for the three different control sites. These curves are depicted in Figure 4.5. 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, 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

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

- Scenario 1. The initial solute concentration in the groundwater is zero, and fertilizer application can vary in space and time.
- Scenario 2. The initial solute concentration in the groundwater is zero and fertilizer application is restricted to be the same for all 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. A planning horizon is the number of successive years that fertilizer is applied, after those years no more fertilizer is applied.

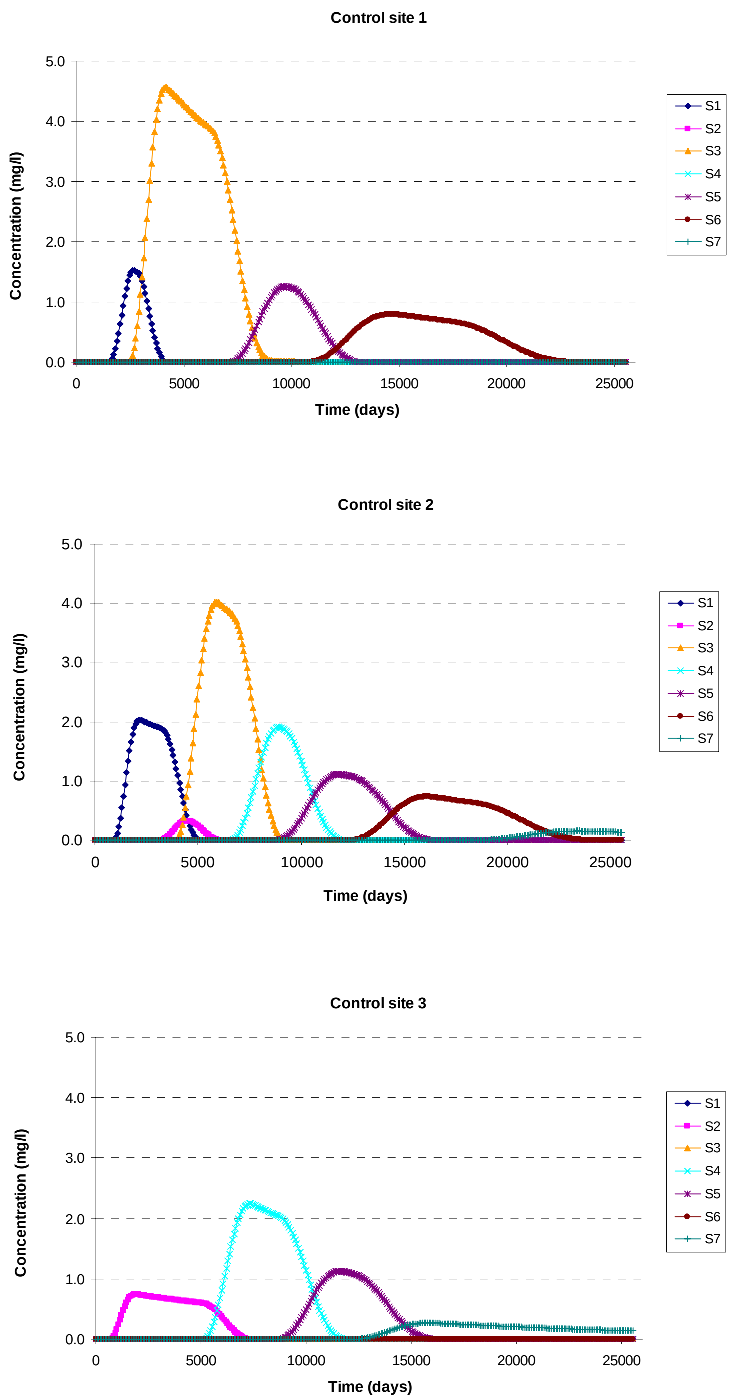


Figure 4.5 Breakthrough curves for the control sites

4.2.3 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 total optimal fertilizer application would be the same (3731 ton/year on average), an equal annual benefit (20.96 M€/year) would be obtained. In Table 4.3 this values are shown. The total benefits were calculated considering the sum of all the profits of each source times its cultivated area. The breakthrough curves for the control sites are shown in Figure 4.6.

Table 4.3 Maximum nitrate concentrations for maximum benefits. Scenario 0

Planning horizon (years)	Maximum concentration (mg/l)	Total Benefits (M€/year)
10	34.6	20.96
20	54.8	20.96
30	61.7	20.96
40	64.0	20.96

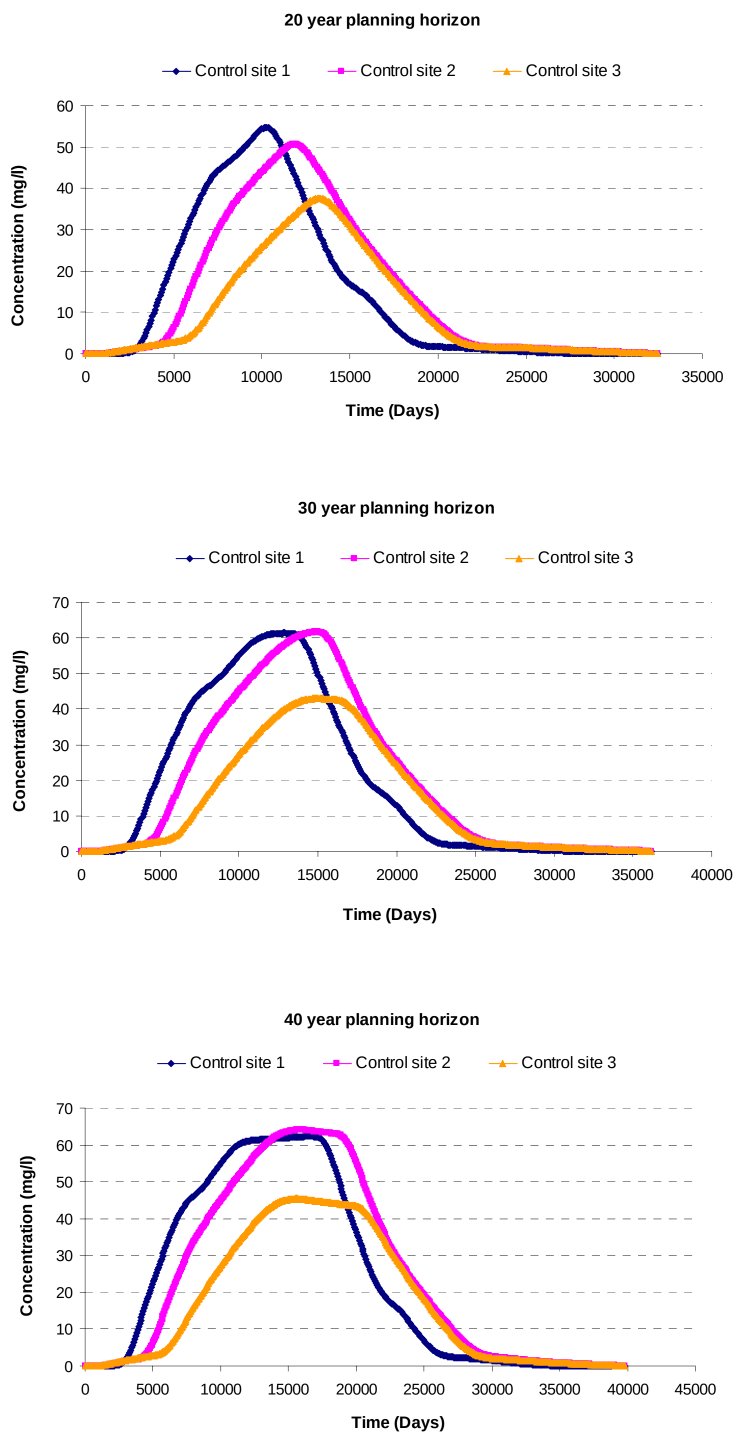


Figure 4.6 Breakthrough curves. Scenario 0

4.2.4 Scenario 1. Variable fertilizer application

For the 10 year planning horizon, the fertilizer application was the same as that providing the maximum benefits (Table 4.4), 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.

Table 4.4 Fertilizer application that maximizes the total net benefits

Source	Fertilizer Application (kg/ha)
S1	58.2
S2	134.1
S3	181.4
S4	207.2
S5	263.1
S6	58.2
S7	134.1

Figure 4.7 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. The results for the 40 year planning horizon are representative of long-term management.

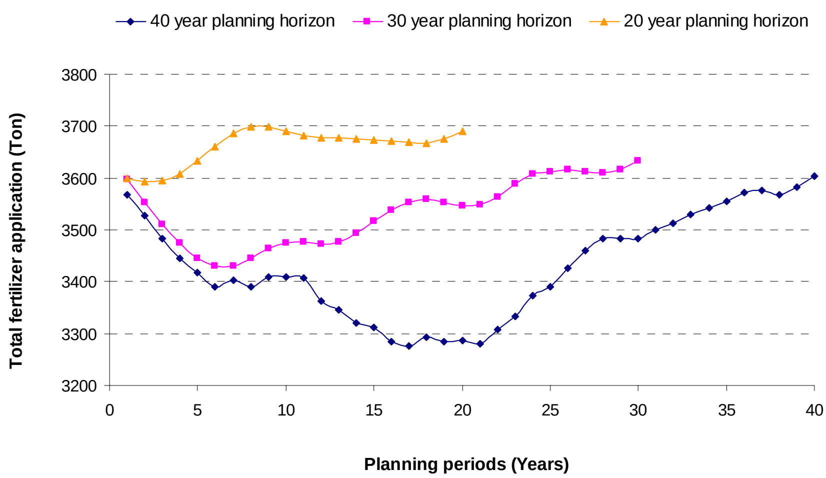


Figure 4.7 Total fertilizer application for different planning horizons. Scenario 1

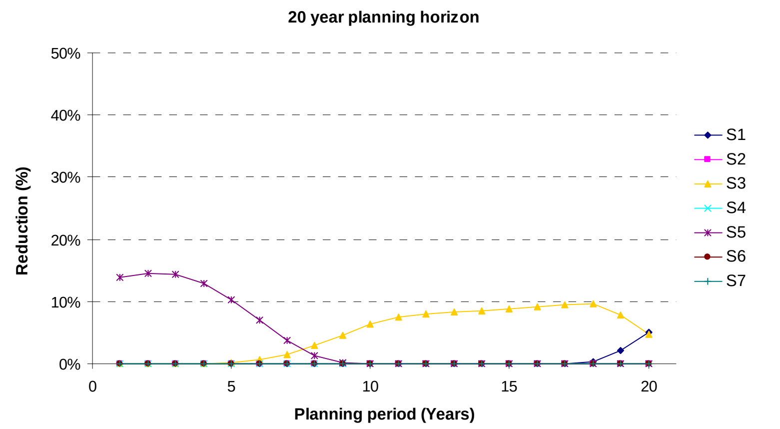
For the 20, 30 and 40 planning horizons the fertilizer application has to be reduced in order to maintain the nitrate concentrations below 50 mg/l. Figure 4.8 shows the reduction of fertilizer application corresponding to each source with regards to the fertilizer application of maximum crop yield. The 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. As it can be seen, the application is further reduced as the planning horizons increases. Groundwater nitrate concentration becomes higher as the fertilizer is applied for more years.

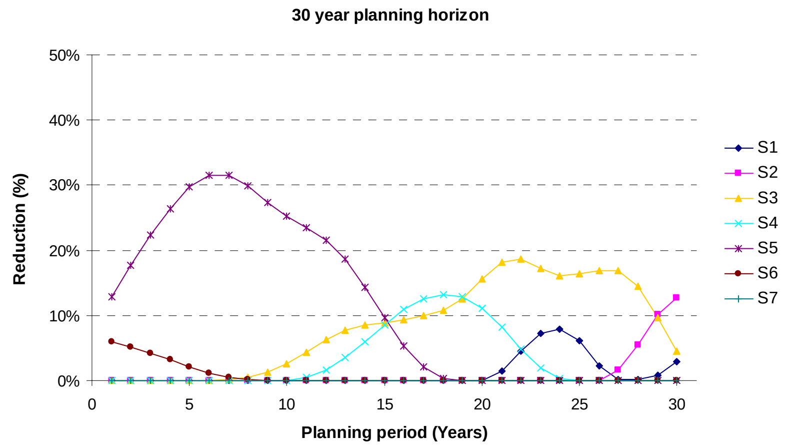
According to Figure 4.8 for the 40 year planning horizon, crop area *S5* (corn) requires the most fertilizer reduction, reaching a 30% reduction during the first 30 years. As shown in Figure 4.5, this crop area strongly influences nitrate concentration at the three sites.

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 4.9 shows the times series of nitrate concentration for the optimal fertilizer application at the three control sites. The arrival time of the peak of the concentration to the control sites is different for each source; therefore the fertilizer reduction is different in time for each source. The maximum value does not exceed the ambient standard of 50 mg/l. As the planning horizons become bigger the peak of the curves also becomes bigger and is practically constant at 50 mg/l.

For the 40 year planning horizon (Figure 4.9) the 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.

The benefits are 20.96, 20.93, 20.83 and 20.76 M€/year for the planning horizons of 10, 20, 30 and 40 years respectively. The longer the planning horizon, the higher the reduction in fertilizer application, with lower average benefits per year.





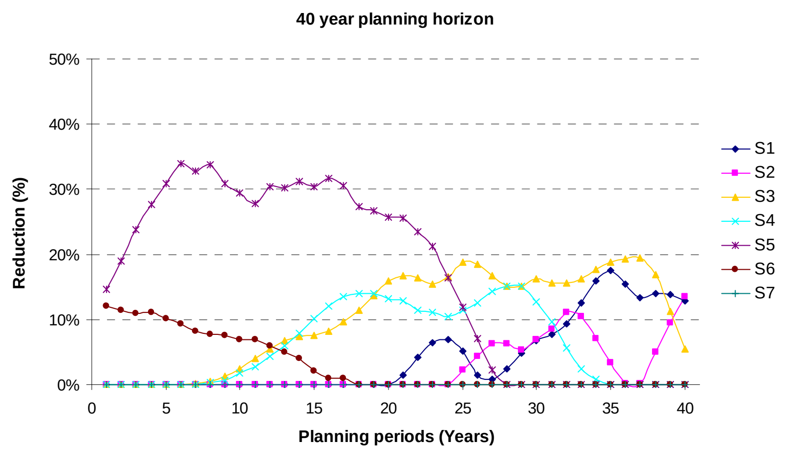


Figure 4.8 Spatial and temporal reduction fertilizer application. Scenario 1

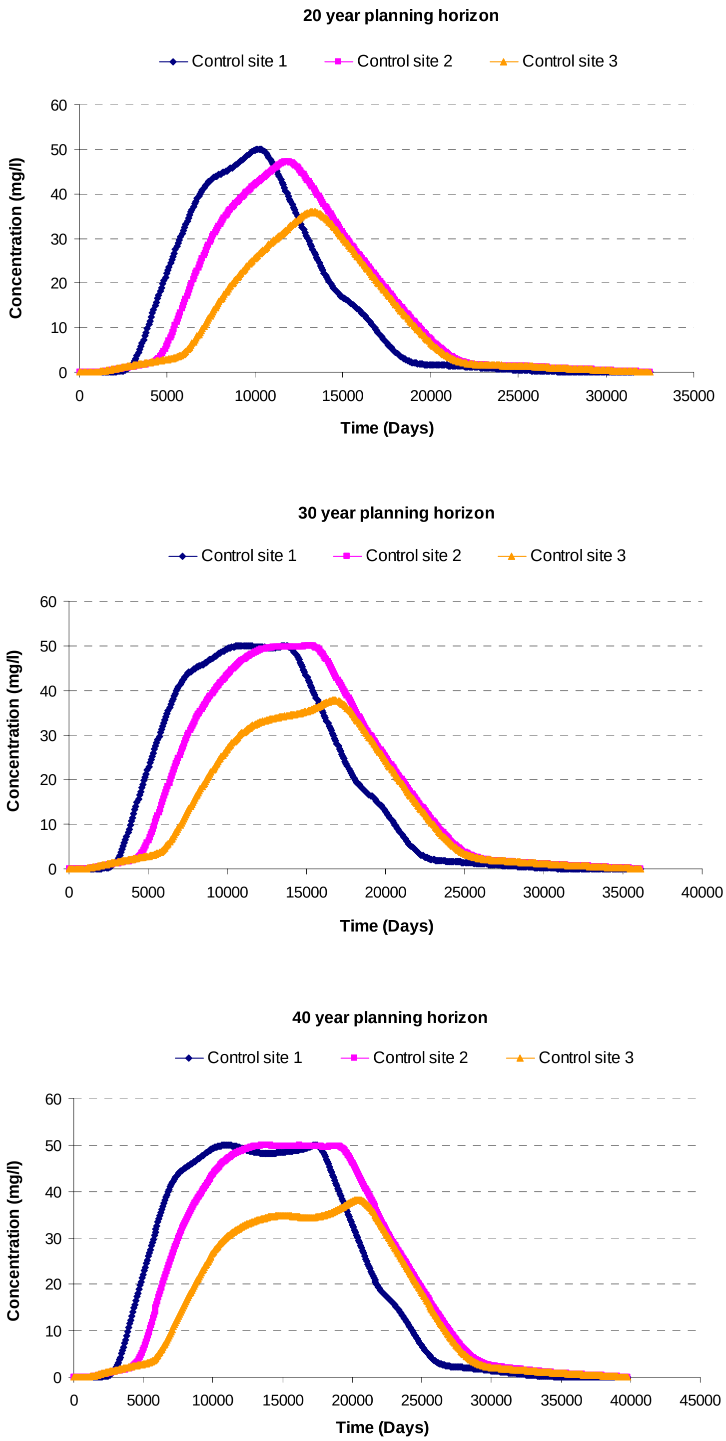


Figure 4.9 Breakthrough curves. Scenario 1

4.2.5 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 4.5 shows the fertilizer application and in Table 4.6 the percentage of fertilizer reduction from the loading that produces the maximum crop yield that is required to meet the ambient standards. The 10 years planning horizon case did not require any reduction; the values are the same as the ones for the maximum profit, which is not the case for the other cases. For the 40 year planning horizon crop area *S5* (corn) again has the highest fertilizer reduction, followed by *S3* (sunflower).

Table 4.5 Constant fertilizer application. Scenario 2

Source	Crop	10	20	30	40
S1	Alfalfa	58.2	57.7	57.7	50.1
S2	Barley	134.1	134.1	126.9	124.1
S3	Sunflower	181.4	164.3	156.1	151.9
S4	Wheat	207.2	207.2	183.3	180.3
S5	Corn	263.1	243.9	194.1	183.7
S6	Alfalfa	58.2	58.2	57.1	55.8
S7	Barley	134.1	134.1	134.1	134.1

Table 4.6 Percentage of fertilizer reduction. Scenario 2

Source	Crop	10	20	30	40
S1	Alfalfa	0.0	0.7	0.8	13.9
S2	Barley	0.0	0.0	5.3	7.5
S3	Sunflower	0.0	9.4	14.0	16.2
S4	Wheat	0.0	0.0	11.6	13.0
S5	Corn	0.0	7.3	26.2	30.2
S6	Alfalfa	0.0	0.0	1.9	4.1
S7	Barley	0.0	0.0	0.0	0.0

Comparing the fertilizer application in scenarios 1 and 2 (Figure 4.10) 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).

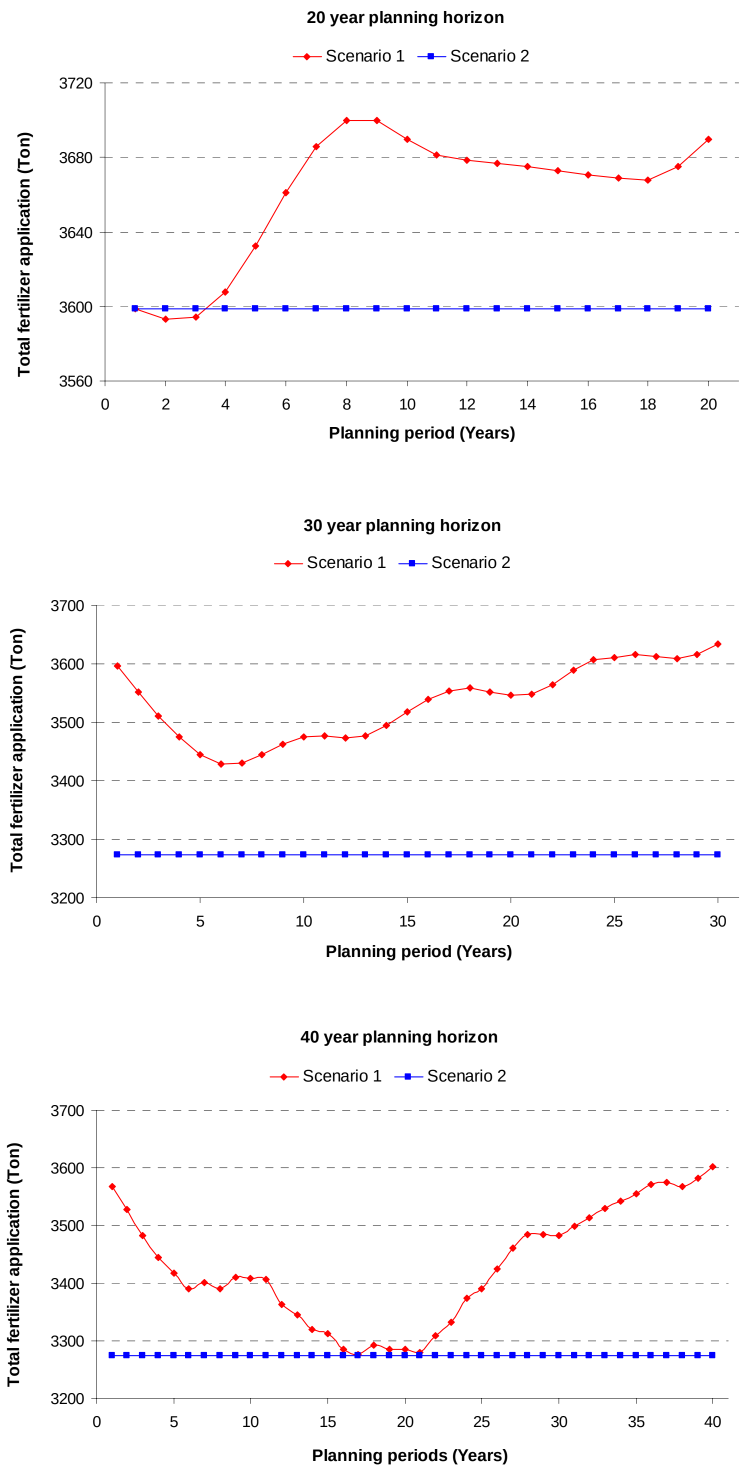


Figure 4.10 Comparison between scenario 1 and 2

In Figure 4.11 the breakthrough curves for the optimal fertilizer application for the 3 control sites are shown. The maximum values does not exceed the ambient standard of 50 mg/l. Comparing Figure 4.9 with Figure 4.11 the maximum concentrations are reached faster in scenario 1 than in scenario 2 and are kept like that longer. In scenario 1, since the fertilizer application can be changed from period to period, it has a better results were the benefits are higher.

In Table 4.7 the average net annual benefits for the scenario 1 and 2 for the different planning horizons are compared. As it can be seen the difference is small, around 1%, while the difference in fertilizer application reduction is approximately 7%.

Table 4.7 Net annual average benefits and total fertilizer application average for Scenario 1 and 2

Planning horizon (year)	Scenario 1 (M€/year)	Scenario 2 (M€/year)	Scenario 1 (kg/ha)	Scenario 2 (kg/ha)
10	20.96	20.96	148.1	148.1
20	20.93	20.90	145.3	142.8
30	20.83	20.68	140.2	129.9
40	20.76	20.58	136.1	125.7

4.2.6 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).

For this scenario it was necessary to simulate the aquifer behavior considering a initial concentration of 55 mg/l, which was applied uniform in the whole aquifer and no fertilizer application. In Figure 4.12 the breakthrough curve for the three control sites is shown, in this figure we can see how the natural attenuation of the aquifer works (wash-out), by the day 1314 (3.6 years) the nitrate concentration in the control sites is 50 mg/l.

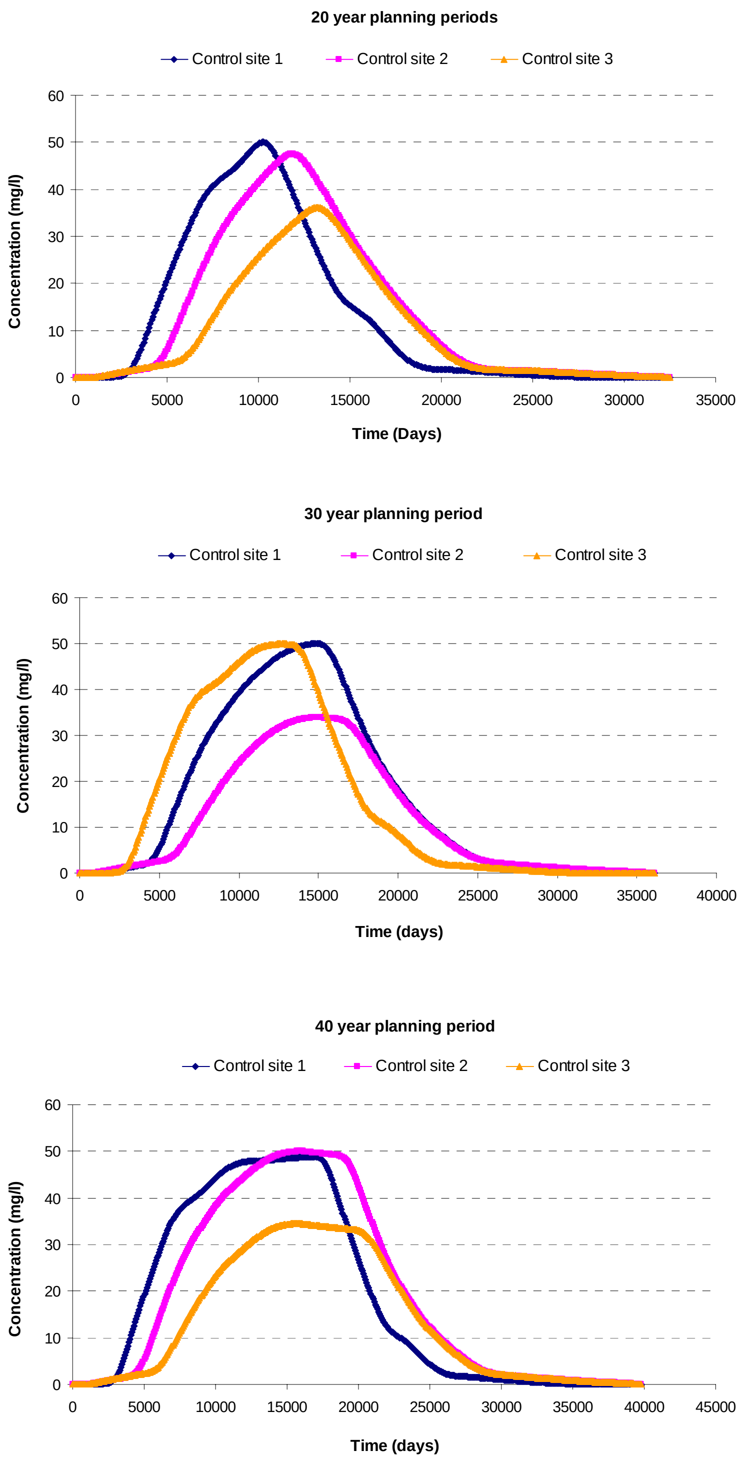


Figure 4.11 Breakthrough curves. Scenario 2

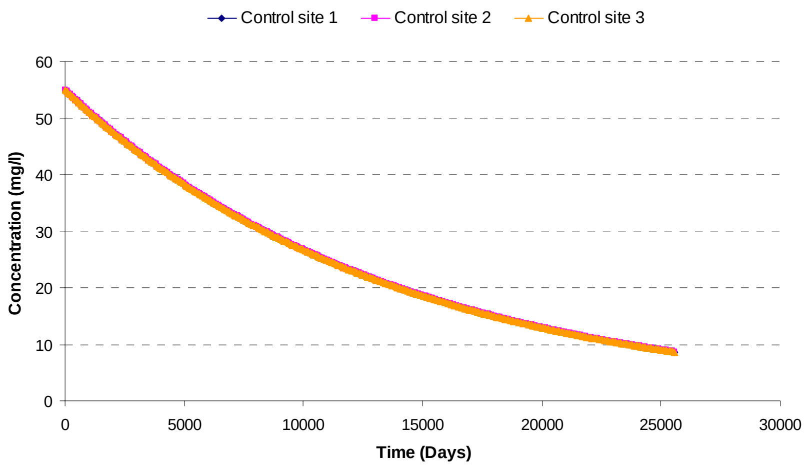
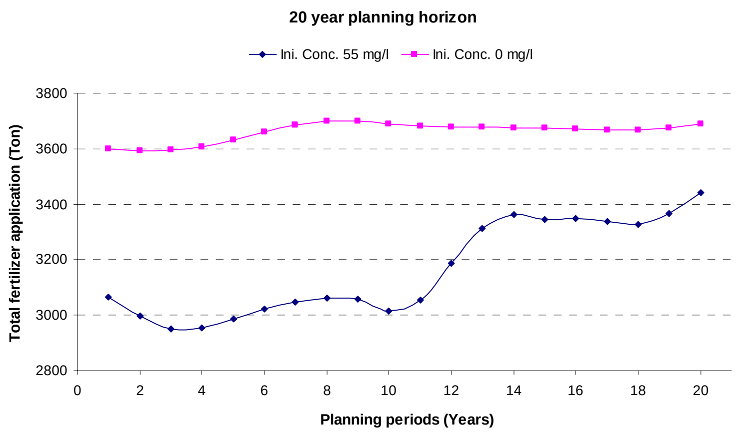
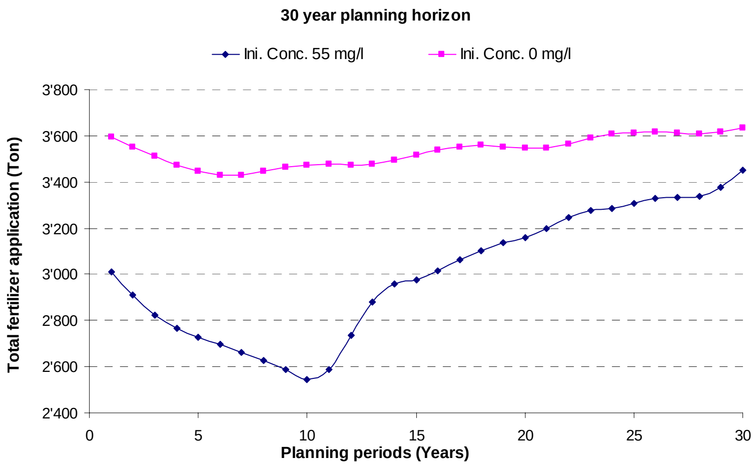


Figure 4.12 Breakthrough curves considering an initial concentration of 55 mg/l. Scenario 3

The recovery time horizons were imposed in the management model by setting the maximum concentration constraint at the specific recovery time and beyond. Figure 4.13 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.

In Figure 4.14 the breakthrough curves for the scenario are shown. In this case the concentration at the beginning of the simulation is the initial nitrate concentration in the aquifer of 55 mg/l. Then after 20 years the maximum concentration is 50 mg/l.





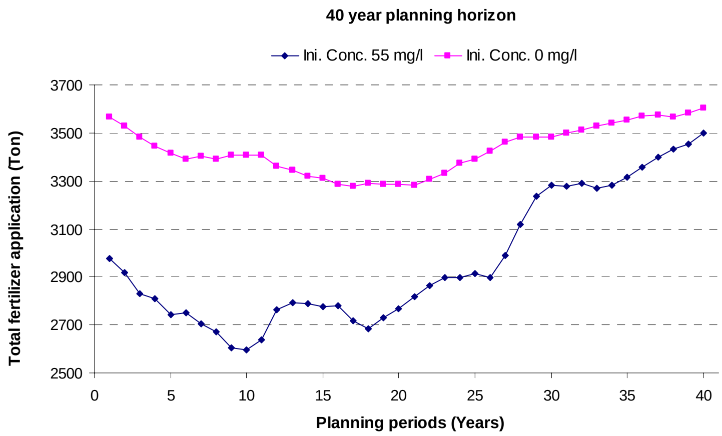
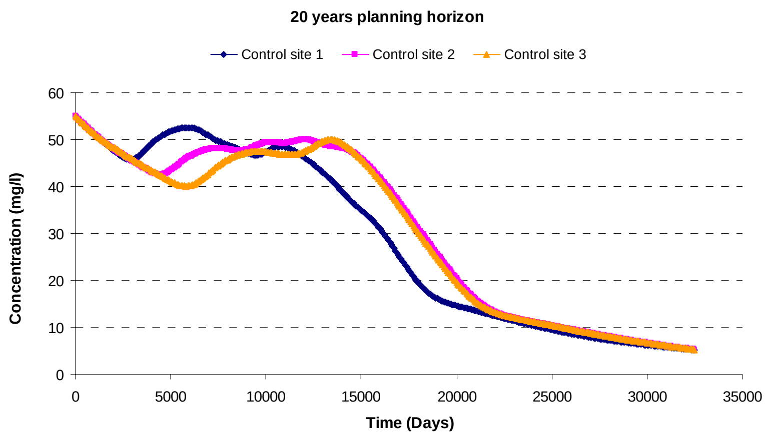
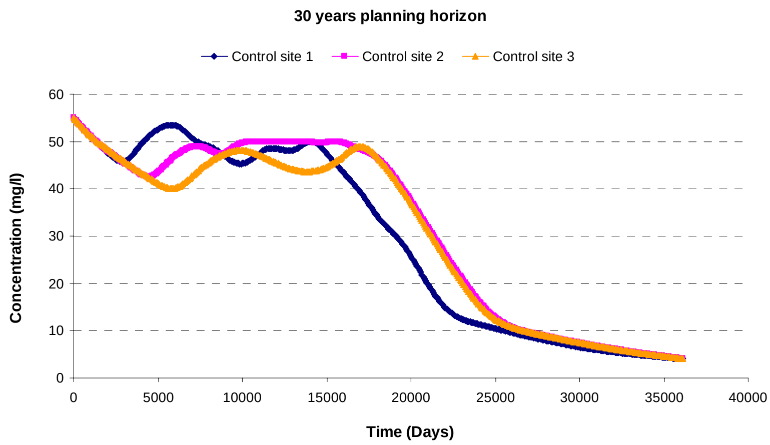


Figure 4.13 Comparison between scenario 1 and 3





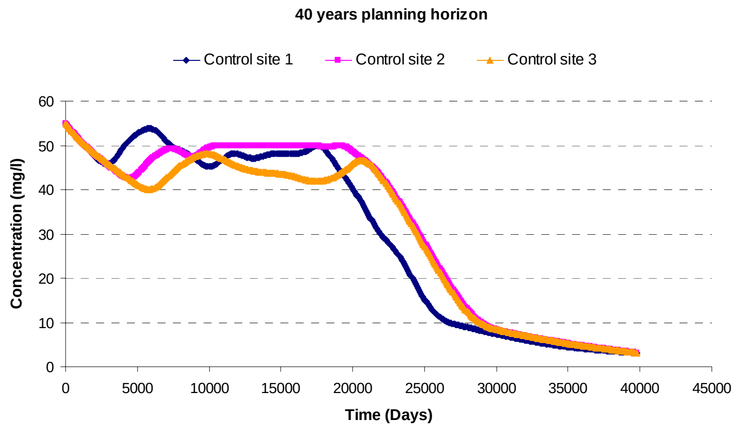


Figure 4.14 Breakthrough curves. Scenario 3 (20 years recovery time)

The ambient standard can be achieved in different times, therefore four different cases were simulated it was considered a 10, 20, 30 and 40 years of recovery time. For this scenario it was used the 40 years management model. And the difference in total benefits is compared.

Table 4.8 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 4.8 Benefits for different recovery times. 40 years planning horizon. Scenario 3

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

Figure 4.15 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.

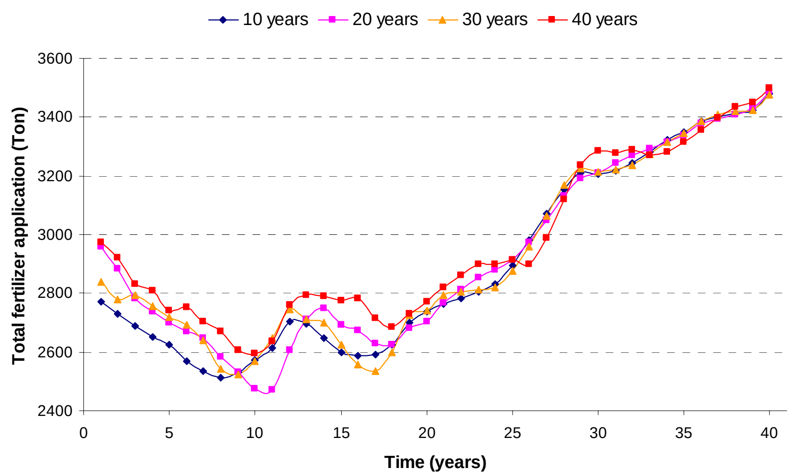


Figure 4.15 Total fertilizer application for different recovery times. 40 management periods. Scenario 3

In Figure 4.16 the breakthrough curves for the control site 2 are compared, and it can be seen when the ambient standard is reached.

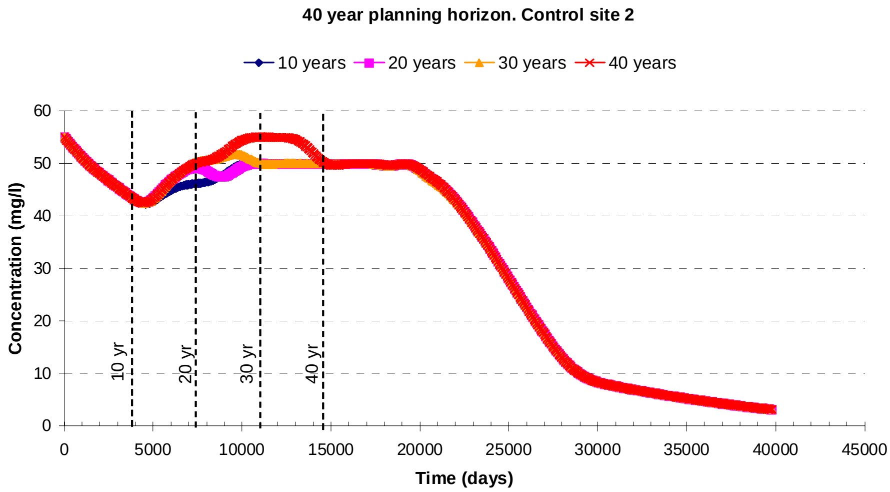


Figure 4.16 Breakthrough curves for different recovery times. Scenario 3

4.2.7 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 horizon case (Table 4.9), 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 (Table 4.10).

Table 4.9 Net annual benefits average and total fertilizer application average for Scenario 3 and 4. 40 year planning horizon

Recovery time (year)	Scenario 3 (M€/year)	Scenario 4 (M€/year)	Scenario 3 (kg/ha)	Scenario 4 (kg/ha)
20	19.45	18.96	115.9	104.7
30	19.53	18.96	115.8	104.7
40	19.66	19.08	117.6	102.5

Table 4.10 Fertilizer application. Scenario 4. 20 management periods

Source	Crop	20	30	40
S1	Alfalfa	57.9	43.3	42.6
S2	Barley	122..3	114.1	114.3
S3	Sunflower	86.3	84.7	87.1
S4	Wheat	149.0	149.2	150.0
S5	Corn	195.4	159.7	146.4
S6	Alfalfa	58.2	58.2	58.1
S7	Barley	134.1	134.1	134.1

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 not just at some control sites. Therefore, the pollutant concentration recharge is implicitly limited to 50 mg/l. The same methodology was simulated and compared with the results previously obtained imposing nitrate concentration limits only at the three control sites. Table 4.11 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), which that this methodology can be very conservative because it doesn't include the nitrate transport in groundwater.

Table 4.11 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

Discount rate

An additional simulation was performed considering the discount rate. The discounting is a key issue when addressing the economics of long-term planning. A high discount rate would in theory favor deferring in time the actions to control the pollution, but since we have the physical constraint of nitrate concentration below the ambient standard, there is no much room for moving large changes. We have done the calculations for scenario 1, comparing the use of fertilizer for discount rates of 0 and 3% (Figure 4.17), where this behavior was observed.

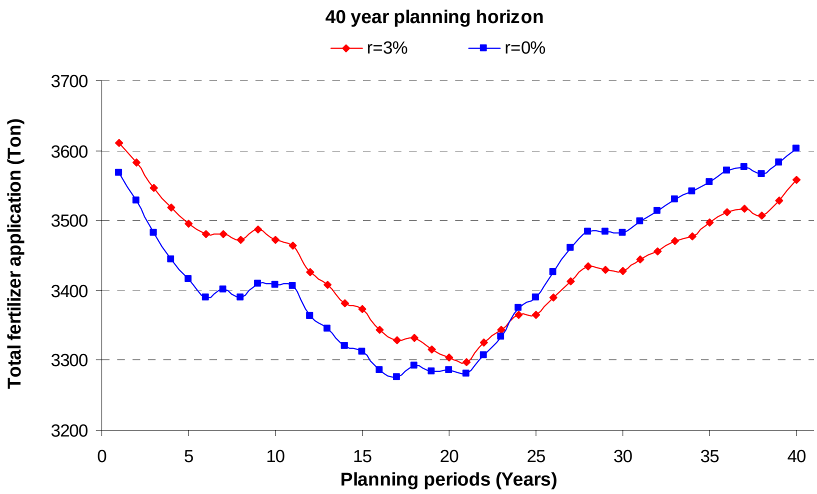


Figure 4.17 Optimal fertilizer application considering a 3% discount rate

4.2.8 Discussion

This chapter has shown the application of the method developed in a synthetic case. The method was applied to an example under four 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 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. For scenario 2 the difference in net benefit for 10 and 40 year management periods is €380,000/year. Taking into account different recovery times (for 40 management periods), the difference in benefits between the more constrained case (10 year recovery time) and the 40 years of recovery is €230,000/year.

In order to accomplish with WFD, water planners have define the quality recovery horizon. The WFD sets 2015 to achieve it, but this deadline can be postponed until 2021 or even 2027 justifying that meeting the 2015 deadline would be disproportionately costly. The simulation results suggest that the costs associated to a 10 year recovery deadline are not disproportionately higher than with 40 year (~9€/ha for scenario 3). This could mean that derogation can not be justified using an economic argument.

Comparing the case of variable fertilizer with a constant application through the planning horizon the benefits are smaller, for example between scenario 1 and 2 the difference in benefits is €180,000/year (40 year planning horizon) The difference in benefits between scenario 3 and 4 is €580,000/year (~23€/ha) which maybe is not to high in comparison to the costs that would have to enforce a complex system where fertilizer use can differ from one year to another, this could justifies the adoption of a constant fertilizer use.

These results are extremely dependent on the aquifer properties. The synthetic aquifer studied herein has very little inertia, since the hydraulic conductivity is relatively high and the thickness is low. The conclusions drawn here could be different for a real aquifer with bigger inertia.

5 Real case study: The Salobral-Los Llanos aquifer

5.1 Overview of study area

In the last 25 years, an important transformation from dry to irrigated lands has taken place in “La Mancha”, a vast elevated plateau (averaging 500 to 600 meters in altitude) located in a semiarid region in central Spain. This transformation has promoted the development of an intensive agriculture that, nowadays, represents one of the main factors in the economic development of the region. In the “La Mancha Oriental” System (MOS), 100 000 ha of irrigated lands equipped with modern technologies are currently settled, regarded as one of the most important in Spain, with most of this irrigation depending on the availability of groundwater. Until the beginning of 2000, more than 1,000 km2 of irrigated cropland and all of the municipalities in the MOS had been supplied solely by groundwater through the exploitation of agricultural and water-supply wells (Martín de Santa Olalla, F. et al. 2003; Sanz et al., 2009). Not surprisingly, the enormous amounts of groundwater abstraction (398 Mm^3/year for irrigation; 8 Mm^3/year for urban supply) are not balanced with the available groundwater resources (323 Mm^3/year; CHJ, 2004). This situation has brought about a progressive drop in groundwater level, by about 80 m in some areas. The MOS has, as its natural drainage in the stretch of the Jucar River between the two reservoirs of Alarcon and El Molinar, whose length is approximately 80 km. Water extraction, which has steadily increased since the 1980s, together with the intense period of drought experienced in recent years, has resulted in a steady decrease of water table levels in the different subzones, with dire environmental consequences, such as the drying up of a significant stretch of the Júcar River in the Summers of 1995 and 1996.

As a result of an intense social, economic, political and environmental debate the farmers together with the administration and society, are currently trying to establish sustainable management for the MOS. Despite confrontations derived from different points of view, all these sectors are convinced of the necessity to preserve such a valuable natural resource as water, especially in this area characterized by a semi-arid climate. Another big concern in the MOS is the increase in nitrate pollution due to the increase of intensive farming and fertilizer use, groundwater nitrate concentrations have reached values of 125 mg/l (Moratalla et al, 2009), far above the 50 mg/l required for drinking water supply. An accurate quantification of nitrate leaching to groundwater is hampered owing to uncertainties in land use practices, on-ground nitrogen loading, groundwater recharge, climate, soil nitrogen dynamics and soil characteristics. The Mancha Oriental System (MOS) is located within the Jucar River Basin which was declared as EU Pilot River Basin in 2002 for the process of the common implementation strategy of the Water Framework Directive

The *"Salobral-Los Llanos"* Domain (SLD) is located in the southeast of the Mancha Oriental System (Figure 5.1 and Figure 5.2) and extends over about 420 km^2. The SLD contains a total population of about 5,000 inhabitants. According to the information from CHJ (2004), 80% of the land is agriculture (337 km^2), from which 100 km^2 are irrigated crops.

The concentration of irrigated crops has induced negative environmental and economic impacts in the area, since the groundwater table has decreased from 60 to 80 meters in the period 1970 to 2002, with an average decrease of about 2.5 to 3 meters per year. The development of the irrigated crops has also led to significant consequences for regional groundwater flow and high nitrate concentrations in the groundwater.

In order to test the method developed in this thesis, the SLD was chosen as case study because it represents a smaller area than the MOS, while showing the same problematic issues as it. Moreover the SLD has a hydrogeologic behavior that is virtually independent from the rest of the MOS.

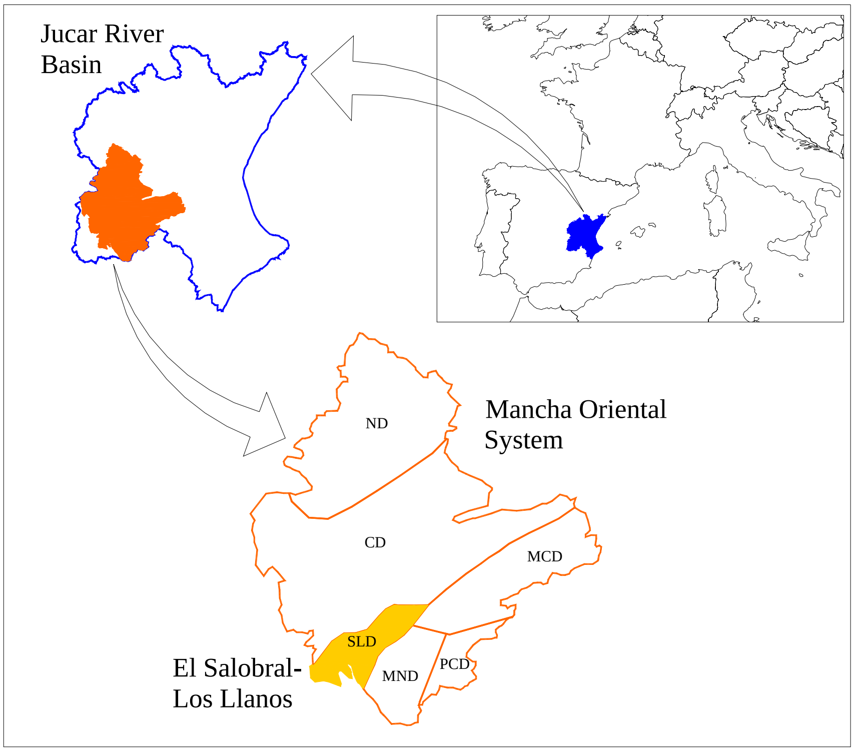
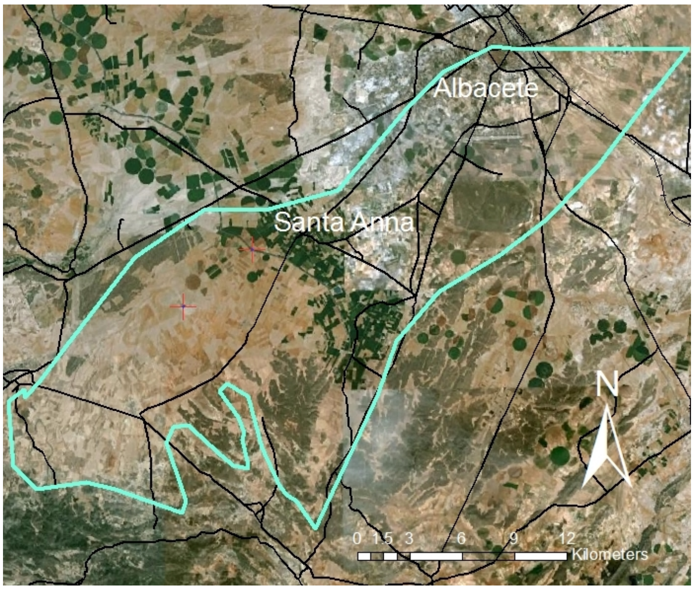


Figure 5.1 Aquifer location

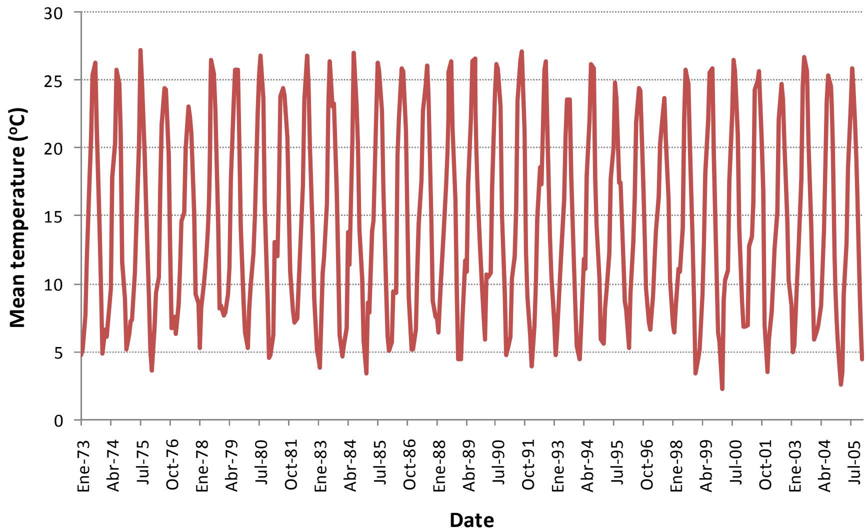


Source: google earth

Figure 5.2 El Salobral- Los llanos domain

Climatology

The region has a mild Mediterranean climate, with dry summers and precipitations in spring and autumn. The climatic conditions of Castilla-La Mancha can be defined as appropriate of a Mediterranean climate, with continental degradation, noticeable fluctuations in daily and seasonal temperatures, and an unequal distribution of scant rains. Semi-arid and with extreme cold winters (under 6°C) and hot summers (above 25°C), the average annual temperatures vary between 13°C and 14.5°C (Figure 5.3), a yearly mean of 2800 hours of insolation. The mean annual precipitation is 362 mm for 1973-2005 (Figure 5.4). The precipitation occurs mainly during autumn, winter and spring, being the rainiest months October, November, May and April.



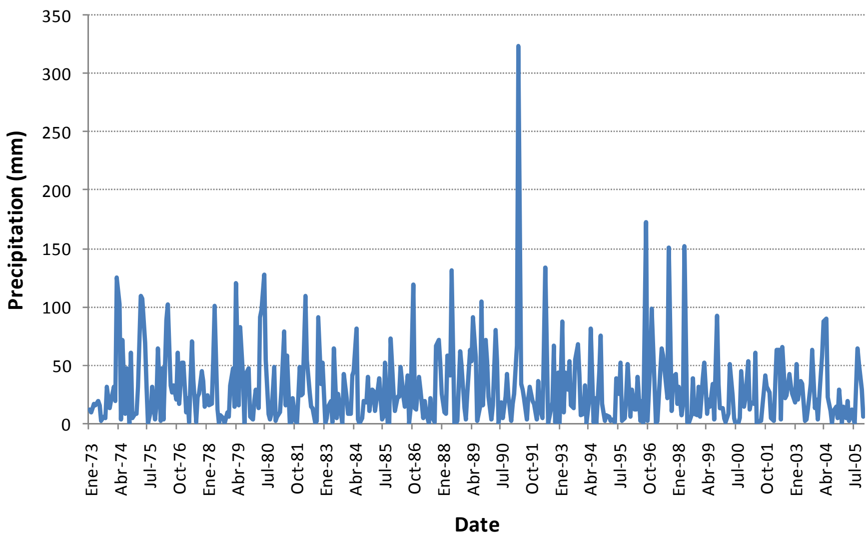
Source: www.meteored.com

Figure 5.3. Mean temperature

Soils

According to the American Taxonomic classification the area is classified as: Order-Inceptsol, Suborder: Ochrepts, Group: Xerochrepts and Suborder: Calcixerollic-Xerochrepts.

The soil characterization has been based on the soil analysis performed in the experimental field "Las Tiesas" reported and reported by Maturano (2002), as shown in Table 5.1. Maturano (2002) pointed out, that taken into consideration that the area is located in a semiarid region the soil shows a medium to low fertility.



Source: www.meteored.com

Figure 5.4. Precipitation

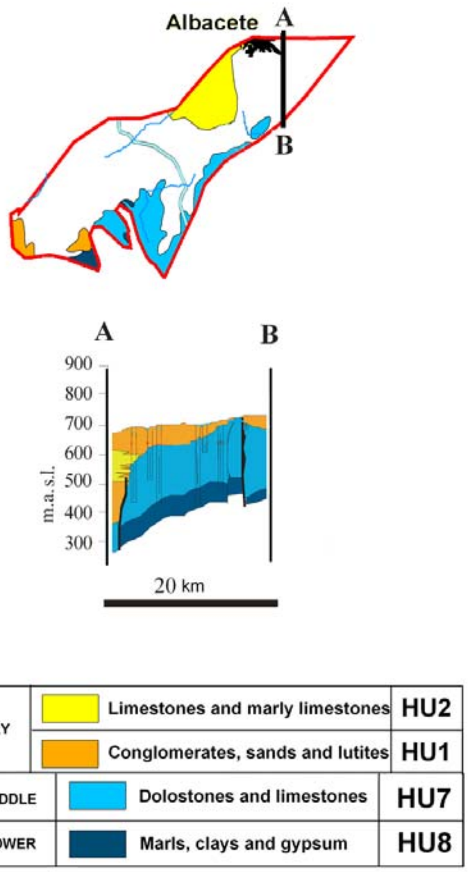
Table 5.1 Soil characterization

Characteristic	Ap	Bk	Ck	C
Depth (cm)	0-25	26-50	51-60	+60
Sand (%)	27	27	76	84
Silt (%)	37	36	18	10
Clay (%)	36	37	6	6
pH	8.39	8.28	8.31	8.35
Electric Conductivity (dS/m)	0.285	0.320	0.433	0.547
Organic Content (%)	1.87	1.52	1.58	0.57
C/N ratio	11	11	11	8
Total N (%)	0.1	0.081	0.083	0.042
Phosphorous assimilable (ppm)	10	2	5	1
Potassium (ppm)	550	295	55	105
Total carbonates (%)	41.18	41.89	71.89	71.59
Active limestone (%)	7.1	7.81	19.17	13.49

Source: Maturano (2002)

Geology

The system is set up by two hydrogeologic units. All groundwater abstraction is from the unconfined hydrogeologic unit 7 (HU7). This unit is made of mid Jurassic dolostones and limestones and can reach 250 thickness (Moratalla et al., 2009). Transmissivity has mean values of roughly 10,000 m^2/day (Sanz, 2005). UH7 is overlaid by a carbonate aquifer unit (HU1) that reaches a maximum thickness of about 75 m. Hidrogeologic Unit 1 is a detrital aquitard. This detrital unit infills a horst and graben structure developed in the Mesozoic basement and shows important lateral changes in facies. This domain is limited by low permeability boundaries which do not allow lateral inflows of groundwater. (Figure 5.5)

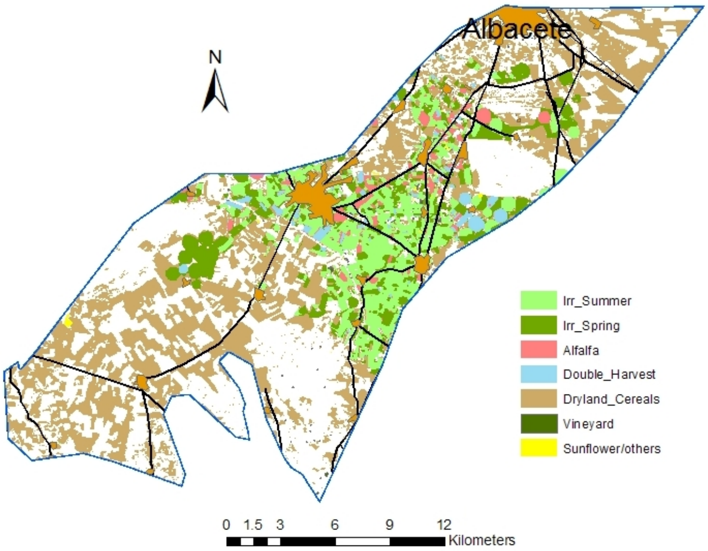


Modified from CHJ (2009)

Figure 5.5 Geologic Map and Cross Section

Crops

The main land use is agriculture, representing 85% of the area. 96 km^2 are irrigated agriculture (Moratalla, 2009). Irrigated crops can be classified into summer (44 km^2), spring (33 km^2) and double harvest (19 km^2) crops, represented mainly by corn, wheat, barley and alfalfa. The number of irrigated hectares has shown a steady increase since the 1980s. In 2005 the total irrigated area was 12,301 ha. The principal crops are show in Table 5.2 (Plan de cultivos 2005). Figure 5.6 shows the localizations of the main crops in 2004, according to the remote sensing techniques. This information was collected from the ERMOT project (Calera et al., 1999, 2003; CHJ, 2006). The images are available from 1982 to 2005.



Source: CHJ, 2006. ERMOT project

Figure 5.6. Main crops in the study area (2004)

The main irrigation users of the Mancha Oriental aquifer are represented by the "*Junta Central de Regantes de la Mancha Oriental*" (JCRMO). This includes not only individual farmers but also Irrigation Communities (CCRR) and "*Sociedades Agrarias de Transformación*" (SATs). These gather individual farmers who share a common irrigation infrastructure, but also includes other uses like public water supply and industries. In total it has 658 members; however, each SAT or CCRR might include each another 150 to 300 individual farmers. Therefore the indirect number of farmers represented by the JCRMO is much higher (Lopez-Gunn, 2003). The JCRMO has been "very proactive in placing complaints against farmers" (Lopez-Gunn, 2003). In the last year sanctions with fines ranging from 300 to 6,010 € (Lopez-Gunn, 2009) were imposed by the JCRMO Water Jury – not the Water Authority – following complaints on non compliance with their Exploitation Plan (Lopez-Gunn, 2009). According to Lopez-Gunn (2003): "Eastern Mancha is an example of rules in use by farmers backed by rules in norm from the Water Authority. There is a clear partnership between the administration and farmers, where increasingly the farmers themselves police their use of water in a devolved system overseen by the Water Administration". Different formulas of stakeholder participation and integrated management in the system have been studied using "Bayesian networks" in the context of an EU project, MERIT (Martín de Santa Olalla, F. et al., 2007).

Table 5.2. Main crops and cultivated area for year 2005

Crop	Area (ha)	%
Corn	3,921	32
Wheat	1,739	13
Barley	1,730	13
Onion	1,329	10
Alfalfa	838	6

Source: Plan de Cultivos

Irrigation, Fertilization and Crop yield

According to ITAP (2005) the recommended irrigation, fertilizer application and crop yield is the one shown in Table 5.3.

Table 5.3. Irrigation for the main crops 2005

Crop	Irrigation (m^3/ha)	Fertilizer (kg/ha)	Crop yield (Kg/ha) 2004
Alfalfa	9,691	20	4,095
Corn	8,375	296	11,100*
Onion	6,350	216	63,789
Wheat	4,580	144	6,986
Barley	3,650	124	6,079

Source: ITAP (2005). *Montoro (2008)

Aiming at the sustainability of groundwater use in the MOS, a management system of the aquifer has been developed taking into account, both supply and demand management, and including the socio-economic and environmental perspectives. An Irrigation Advisory Service was created in 1988 with two main goals: to provide weekly information to farmers about the volume of water to be used for the main crops in the area, and to collect field data about water consumptions and irrigation efficiency. It was observed that for the crops having high or medium to high water requirements farmers use a bit more than the recommended irrigation volumes, about 5%±10% more. Crops with medium to low or low water needs are often cultivated in farms with shortage of water (Martín de Santa Olalla, F et al., 1999).

Current Spatial and temporal distribution of nitrates in groundwater

The highest nitrate concentrations are in the middle part of the aquifer where the irrigated agriculture is located (Figure 5.7). Nitrate concentrations fluctuate from 18.7 to 54.1 mg/l (Moratalla et al., 2009). The lowest nitrate concentrations are 18.7 mg/l, located in forested areas.

Nitrate concentration values shown in Figure 5.7 come from wells for drinking water supply (Moratalla et al., 2009). The highest value was recorded in the well named El Salobral with 54.1 mg/l, exceeding the allowed concentration for human consumption.

Location of higher nitrate concentrations are directly related to the location of irrigated agriculture, which indicates that agriculture, is the major contributor to groundwater pollution. The irrigated area in 1961 was about 29 km^2 (IGME, 1976), in 1976 of 76 km^2 and in 2003 of 96 km^2. The first nitrate analyzes were gathered by IGME during the seventies when the nitrate concentrations were less than 2 mg/l, in 1980 they were about 29 mg/l. The nitrate leaching from soil during the irrigation period or during intense precipitation events and the rate of nitrate transport along groundwater flow may explain the presence of nitrate in groundwater (Moratalla et al., 2009).

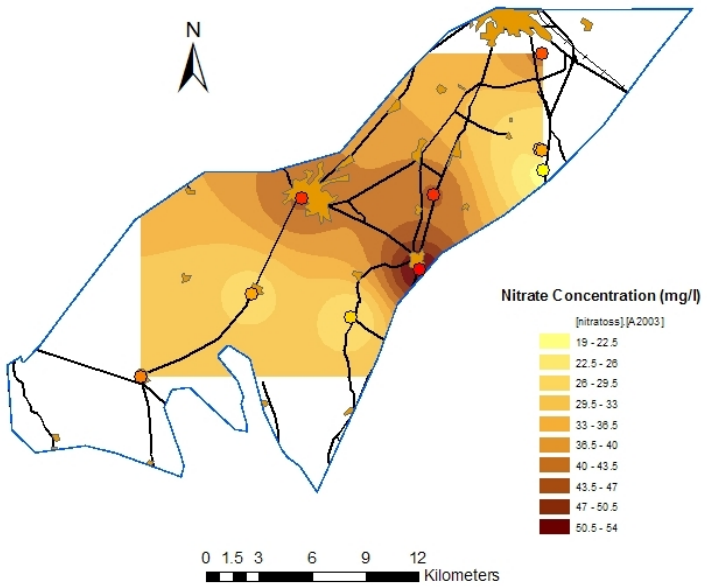


Figure 5.7. Groundwater nitrate concentrations.

The spatial distribution of nitrate in groundwater is also related to the vulnerability grade of HU7; which depends, among other factors, of the depth to the water table, the proximity to the surface of the HU7 tectonic blocks, and the thickness and proportion of fine to coarse-grained deposits in HU1 (Moratalla et al., 2009). HU1 can act as a barrier to pollutants because it consists of a significant thickness of lutites and fine sands. In this sense, the down-dropped blocks of HU7 are less affected by both point and non-point pollution sources. On the other hand, uplifted blocks are more vulnerable to groundwater pollution since they are closed to the surface and they are covered by relatively thin detritic deposits.

5.2 Agronomic modeling

In order to obtain the production functions several simulations were performed with GEPIC for different water and fertilizer applications for each crop. The GEPIC model uses six types of input data (Liu et al., 2007):

- Information on location (latitude, longitude, DEM and slope).
- Climate data.
- Soil physical parameters,
- Land use data.
- Plant parameters.
- Management data, such as irrigation and fertilizer application.

The data used for the agronomic modeling (see Liu et al., 2007) was provided by the Swiss federal Institute for Aquatic Science and Technology. Briefly, the DEM data was obtained from the 1km resolution (30”) digital elevation model GTOPO30 of the United States Geological Survey (USGS) (EROS Data Center, 1998). Terrain slopes are from the 1-km resolution (30”) HYDRO1K digital raster slope map (USGS, 2000). The daily maximum and minimum temperatures and precipitation data were derived from the Global Daily Climatology Network (Gleason et al., 2002)[6]. The EPIC specific monthly statistical climate data were estimated based on the daily climate data. Average daily relative humidity, sunshine hours, and wind speed per month were taken from the FAO CLIMWAT database (FAO, 1993). Solar radiation was estimated from sunshine hours. The climate parameters of each grid are assumed the same as those in the ‘‘closest’’ climate stations. The boundary of a region within which all the grids share the same set of climatic variables was created with a method of Thiessen Polygons.

A minimum of seven soil parameters is required for simulation: depth, percent sand, percent silt, bulk density, pH, organic carbon content, and fraction of calcium carbonate. Soil data of depth and texture (percent sand and silt) was obtained from the Digital Soil Map of the World (FAO, 1990). Soil pH, organic carbon content, and calcium carbonate fraction are from ISRIC-WISE International Soil Profile Data Set (Batjes, 1995).

[6] Daily climate data from 1994 to 2004 is downloadable from the website of the National Climate Data Center (NCDC) (www.ncdc.noaa.gov).

Bulk density was calculated by a pedotransfer function (Saxton et al., 1986) based on the thickness and texture in each soil layer. Crop calendar data was obtained from FAO (2005), which provides the data for 90 countries.

A difficulty inherent in simulation models is that coefficients and processes must be calibrated to reflect local conditions. Such calibration is essential as it ensures that results are applicable to the region of interest. Proper calibration of EPIC is complicated by the lack of local data on nitrate leaching. Some of the EPIC specific parameters regarding nitrogen leaching were not explicitly calibrated in this study; however, the results are consistent with some values reported in literature (Martinez et al., 2004; Basso and Ritchie, 2005). The coefficients of quadratic functions representing the crop yield and leaching are shown in Table 5.4 and Table 5.5, and the graphs showing the response of fertilizer and water application on crop yield and nitrate leached is shown in Appendix A (Figures A.1 – A.20).

Table 5.4 Production functions

Crop	a	b	c	d	e	f
Wheat	8.53e+02	1.50e+01	-2.30E-02	4.66E+01	-1.32E-01	-1.90E-02
Corn	2.91E+02	2.24E+01	-1.80E-02	3.43E+01	-6.60E-02	1.10E-02
Barley	1.84E+03	4.31E+00	-1.10E-02	4.23E+01	-1.39E-01	1.40E-02
Alfalfa	-1.89E-12	2.72E+01	-1.40E-02	2.45E+02	-1.28E+00	-1.62E-01
Onion	2.31E+04	1.71E+02	-3.05E-01	-1.6E-07	-8.45E-01	7.34E-01

Table 5.5 Leaching functions

Crop	g	h	i	j	k	l
Wheat	-2.28E+01	2.05E-01	-2.46E-04	1.97E-01	8.13E-04	-5.31E-04
Corn	-5.95E+00	8.30E-02	-9.82E-05	1.90E-02	6.66E-06	4.93E-04
Barley	3.40E+00	8.30E-02	-2.27E-04	-2.10E-02	5.23E-04	7.52E-04
Alfalfa	-1.07E-09	2.70E-02	-1.89E-05	-2.67E-01	6.00E-03	1.84E-04
Onion	-1.03E+01	4.50E-01	-2.76E-05	9.25E-09	4.51E-04	2.73E-04

5.3 Groundwater flow modeling

Several studies have been conducted in the Mancha Oriental System (MOS) and four different groundwater flow conceptual models have been proposed (IGME, 1984; DGOH, 1988; Font, 2004 and CHJ, 2009). The most comprehensive is the last one conducted by "*Confederación Hidrográfica del Júcar*" (CHJ, 2009). Most of the data used in building the new groundwater model for "El Salobral" was obtained from that model.

The groundwater flow model was developed using the finite-difference code MODFLOW (McDonald and Harbough, 1988).

Model domain and discretization

The study area was discretized by dividing it into 60 rows and 82 columns; the grid spacing was 500 meters. The study area is located between the X-coordinates: 570,000 - 611,000; and Y-coordinates: 4,288,000 - 4,318,000. The model has 3 layers representing the 3 main units of the system, being the deepest the main aquifer. The model is solved with monthly time steps for 1975 to 2005 conditions.

Initial conditions

The oldest piezometric data is from 1975, and it was considered that they represent the initial conditions, of the system. In Figure 5.8 the piezometric heads for 1975 are shown being around 700 meters above sea level in the south-west part and 665 meters in the north-east; therefore, the original flow direction was from south-west to north-east.

Flow boundary conditions

The aquifer is bounded in all direction by low permeability conditions except for the northern area. The northwestern boundary comprises the low-permeability Multiple Fracturation Line (Sanz et al., 2009). The southeastern boundary corresponds with the NE-SW area of *"El Salobral-Peñas de San Pedro"* Fault (SSF), which does not allow any groundwater flow between the SLD and *Moros-Nevazos Domian* (MND), and the southern boundary coincides with the termination of the *Pozohondo* fault and the outcropping of the HU8 (Sanz et al., 2009).

According to the flow direction and the piezometric information we approach the the north part of the aquifer with a constant head boundary representing a subsurface out-flow.

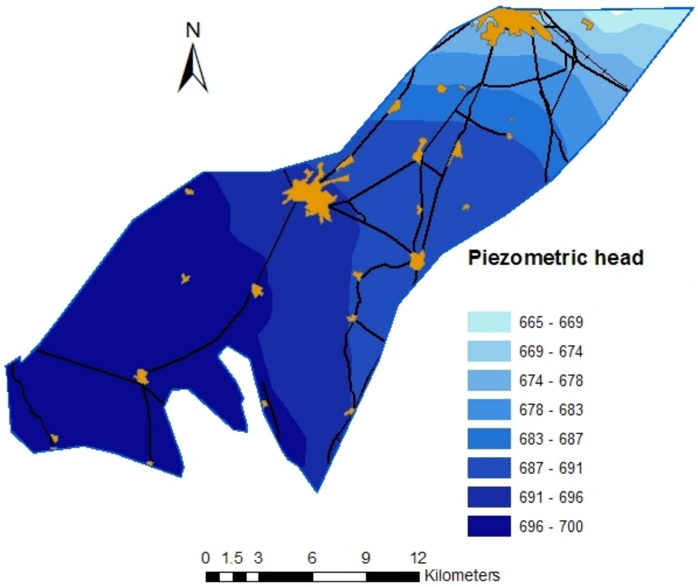


Figure 5.8 Piezometric head for 1975

Hydraulic parameters

The values of transmissivity, specific storage and specific yield were taken from Sanz's PhD. dissertation (2005) and are shown in Table 5.6. In order to calibrate the model these values were adjusted.

Table 5.6 Hydraulic parameters

Hydrogeologic Unit	Transmissivity (m^2/day)	Ss (1/m)	Sy
HU1	1,000-7,000	1e-5 – 1e-4	0.2 – 0.008
HU4	1-50	1e-5	0.2 – 0.06
HU7	2,000-30,000	1e-5 – 9e-5	0.088 – 0.04

Groundwater recharge

The groundwater recharge due to rainfall was taken from CHJ (2009). The recharge values are homogenously distributed in five different areas for the period 1940 to 2001. From 2001 to 2005 the values were taken from the results of the model *Hidromore* model (Calera et al. 1999, 2003). Another source of recharge is the surface water used for irrigation taken from the Tajo-Segura channel as part of a program to reduce groundwater extraction (groundwater substitution).

Groundwater withdrawal

The groundwater withdrawal was taken from CHJ (2009). In this study the values were taken from two different sources. From 1975 to 2001 the values were estimated taking into account the crop water needs and the cultivated areas of each crop. The values from 2001 to 2005 were estimated with remote sensing techniques, as explained in Castaño (1999) and Calera et al. (1999).

In 2001 some boreholes that fed a network of irrigation channels built in the 60's in the Salobral-Los Llanos zone (that had experienced a groundwater level drop up to 70m) were closed, and the system begun to receive 15 Mm^3 /year from the Tajo-Segura transfer channel. This has allowed a certain stabilization of groundwater levels in this zone. The plan is to implement this measure in other zones and increase the use of surface water up to 80 Mm^3/year, so that abstraction does not exceed available resource.

In 2003, water supply for Albacete city formerly was provided by a group of wells in the South of the city, was substituted with surface water coming from the Alarcon reservoir (Júcar river). Although the main reason for this measure was the poor drinking quality of groundwater, it has had a positive impact on the quantitative status by reducing groundwater demand in some 8 Mm^3/yr. (UCLM, 2006)

Flow model calibration

The model calibration involves determining the magnitude and spatial distribution of the model parameters that better reproduce the observed values. The piezometric information measured in 21 wells (Figure 5.9) from 1975 to 2005 was calibrated against the calculated heads in the aquifer. The hydraulic parameters were adjusted for the best fit of the calculated heads to the observed ones. Not all of the 21 wells had information the whole period only 10 that are shown in the appendix B (Figure B.2 to B.12). In Figure 5.10 the calculated and observed head for the well 882 is shown, this well is of importance because the effects of the well substitution can be observed from 2002 to 2005 the groundwater levels are stabilized. This effect is only observed in the well.

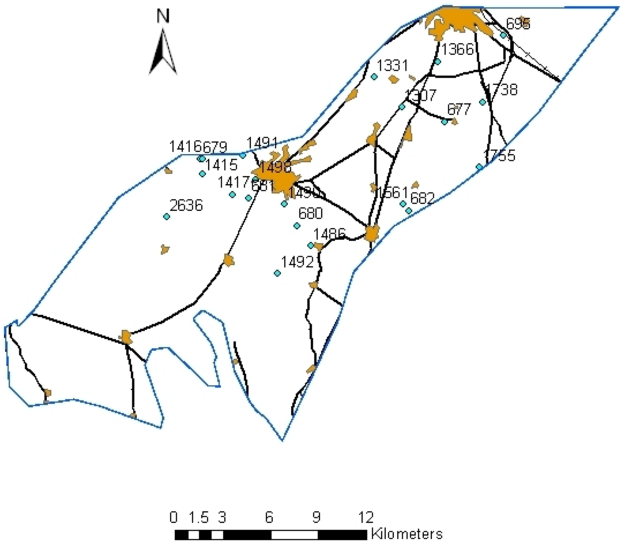


Figure 5.9 Observation well location

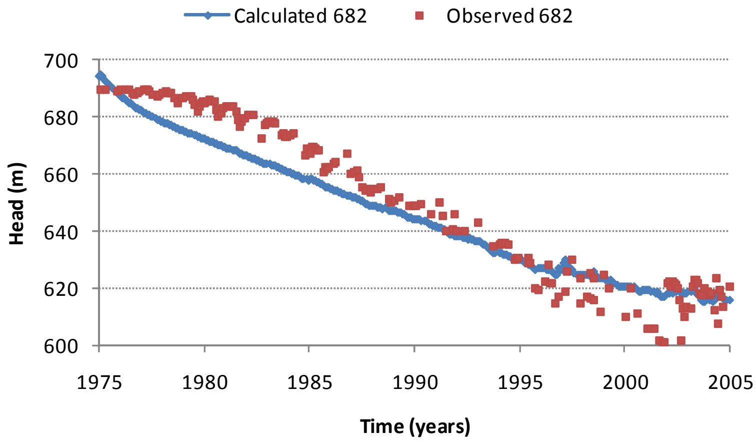


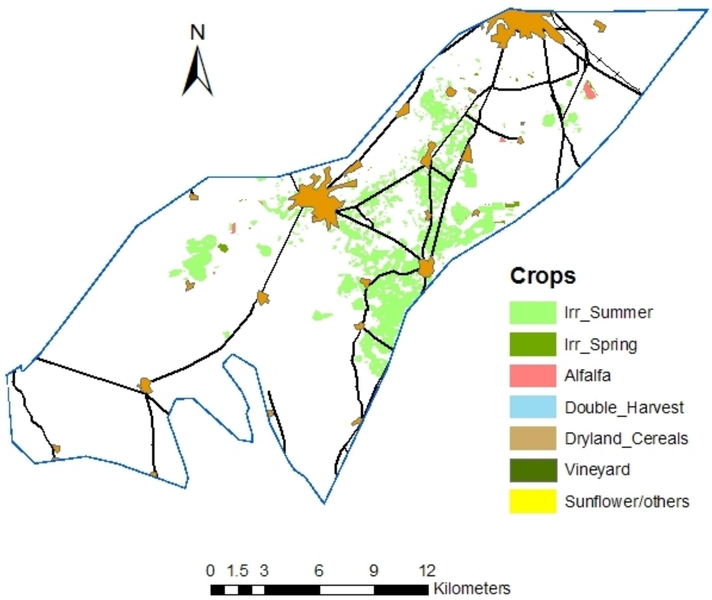
Figure 5.10 Observed vs calculated heads. Well 682

5.4 Groundwater nitrate transport modeling

In order to formulate the nitrate transport model, it was necessary to determine the pollution areas and the nitrate load inputs.

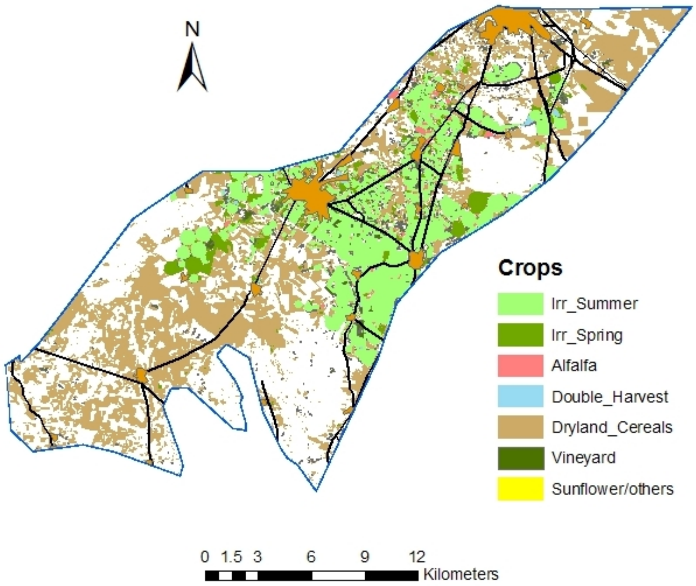
The nitrate loading areas were defined using remote sensing images. Two different areas were considered; the 1982 crop area was used for the period from 1975 to 1985, and the 1989 area was used from 1986 to 2005. Figure 5.11 and Figure 5.12 show the crop areas for those years. These images were chosen because there is an important change in area after 1989, but from 1989 to 2005 the cultivated area stayed more or less constant.

In order to estimate the nitrate input loads, the quadratic functions of Table 5.4 and Table 5.5 were used. Once the optimal fertilizer use and nitrate leaching that maximize the crop yield were obtained, the parameters were adjusted to the best fitting to the values simulated in GEPIC. To calibrate the model, the fertilizer had to be slightly increased from the optimal values, what is in accordance with Ramos et al. (2002). They mentioned that N inputs in the Valencian Community are higher than the values recommended by some researchers, and that nitrate values were in most cases within the range of 150-300 kg N/ha. The nitrate loads used were the ones shown in Table 5.7.



Source: CHJ, 2006. ERMOT project

Figure 5.11 Crops area in 1982



Source: CHJ, 2006. ERMOT project

Figure 5.12 Crops areas in 1989

Table 5.7 Nitrate leaching

Crop	Nitrate leaching (Kg/ha)
Alfalfa	15
Corn	116
Onion	94
Wheat	44
Barley	52
Dryland	20

Few data was available to conduct a real calibration. Only 10 observations wells were available with 1 data point per year, from 1998 to 2004. The calibration was done adjusting the nitrate loads as mentioned above. Figure 5.13 shows the simulated nitrate concentrations for 2005.

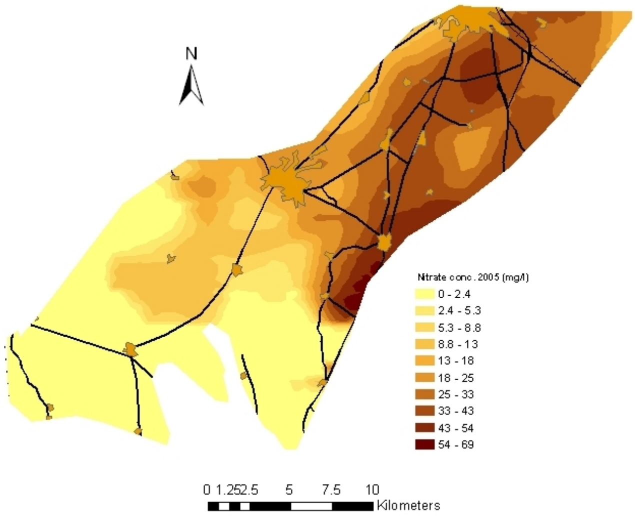


Figure 5.13 Calculated nitrate concentrations. 2005

5.5 Hydro-economic management model

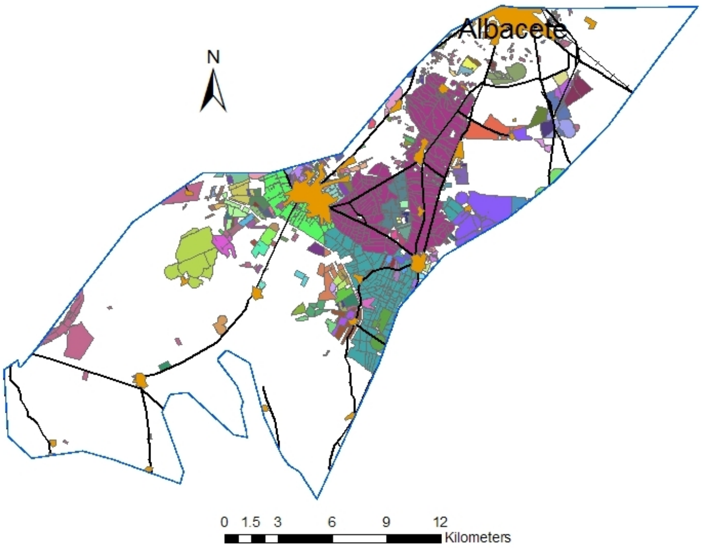
The model considers a planning horizon of 50 years in which the fertilizer application remains constant . The irrigation water applied was kept constant at the level in which the crop yield is maximum. The fertilizer and crop prices were taken from the ITAP[7] (Instituto Técnico Agronómico Provicial de Albacete)

The groundwater flow and nitrate transport simulation was extended until the year 2300, when all the concentration peaks already passed by all the observation wells, in order to derive the concentration response matrix.

5.5.1 Concentration response matrix

The first task in developing the concentration response matrix was the delimitation of the main crop areas or pollutant sources. Two criteria were taken into account: the type of crop and the administrative distribution of the crop fields. Figure 5.14 shows the administrative areas; there are 150, but 11 main areas can be distinguished (Figure 5.15). These crop areas were taken as a starting point in defining the pollutant source areas, once subdivided taking into account the main crops and the surface area information from remote sensing. Finally, 12 areas were selected, shown in Table 5.8 and in Figure 5.16 in which the number represents the administrative area and the letter is the kind of crop (for example 11c, is corn located in the administrative area 11).

[7] www.itap.es



Source. JCRMO (2005)

Figure 5.14 Administrative areas for irrigation management

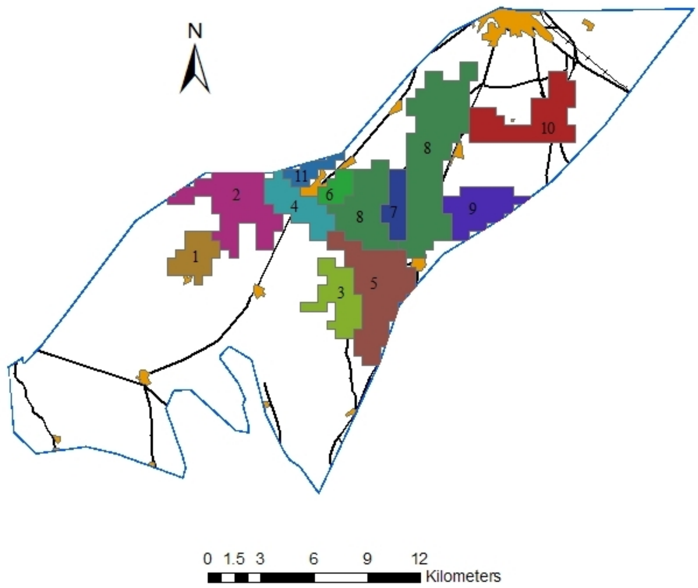


Figure 5.15 Discretization of administrative areas

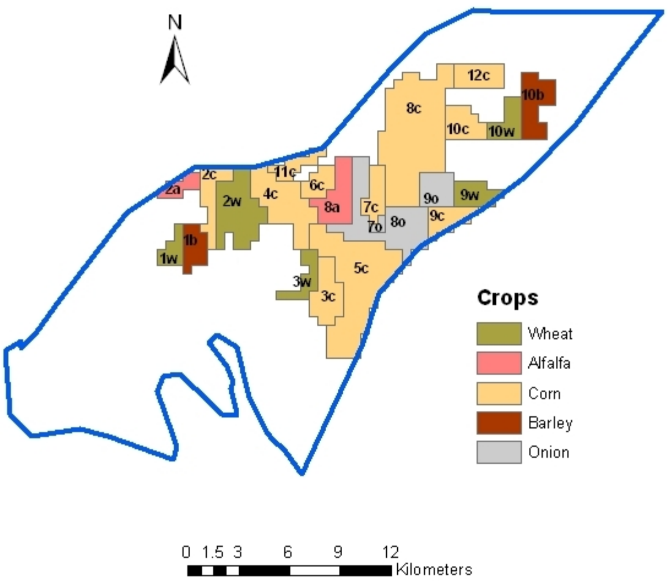


Figure 5.16 Crop type subdivision

Table 5.8 Crop areas

Area	Corn (ha)	Wheat (ha)	Barley (ha)	Onion (ha)	Alfalfa (ha)	Total (ha)
1		271	331			602
2	463	849			232	1,544
3	519	280				799
4	736					736
5	1,750					1,750
6	296					296
7	366			75		441
8	1,990			1,142	553	3,685
9	245	406		195		846
10	391	345	414			1,151
11	326					326
12	450					450
TOTAL	7,533	2,151	745	1,412	784	12,626

Once the crop areas were defined, the concentration response matrix was developed by simulating nitrate concentration at the control wells for a unitary fertilizer application at the crop area. The simulation time horizons were determined by the time for which the peak solute concentration completely passed the control sites. The simulation was done until the year 2300. Breakthrough curves were obtained for each crop area and for the ten different control sites, as shown in Figure 5.17. The majority of these control sites correspond to current well fields for drinking water supply. Only control sites *sondeo 8* and *sondeo 9* are not supply wells, but are selected in order to control nitrate concentrations at different locations within the groundwater body.

Figure 5.18 shows the curves generated by the crop area 8c. This crop area shows a bigger influence on the control site "sondeo 9". Each crop area has different influence over the different observation wells, as shown in appendix C (Figures C.1 – C.12). Therefore, some of them have a very small influence upon the concentration in the control sites as 11c, 10w, 10b and 2a. The crop areas whose resulting peak groundwater nitrate concentration arrive the latest to the control wells are 1w and 1b; they have a very small influence on the final nitrate concentration.

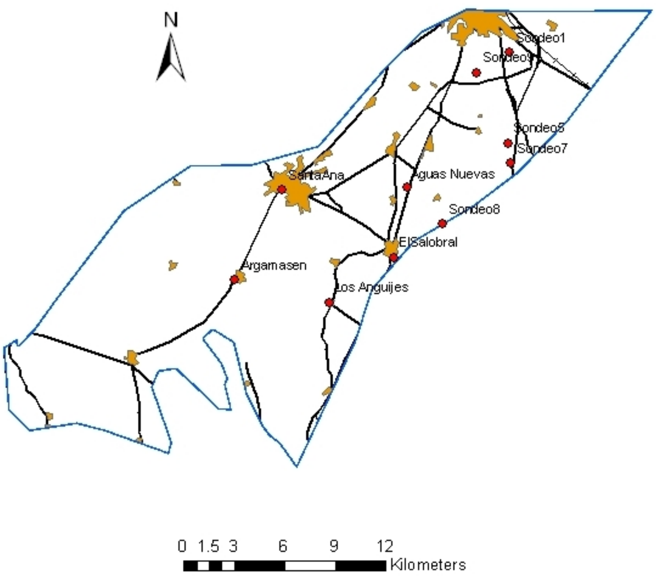


Figure 5.17 Control sites location

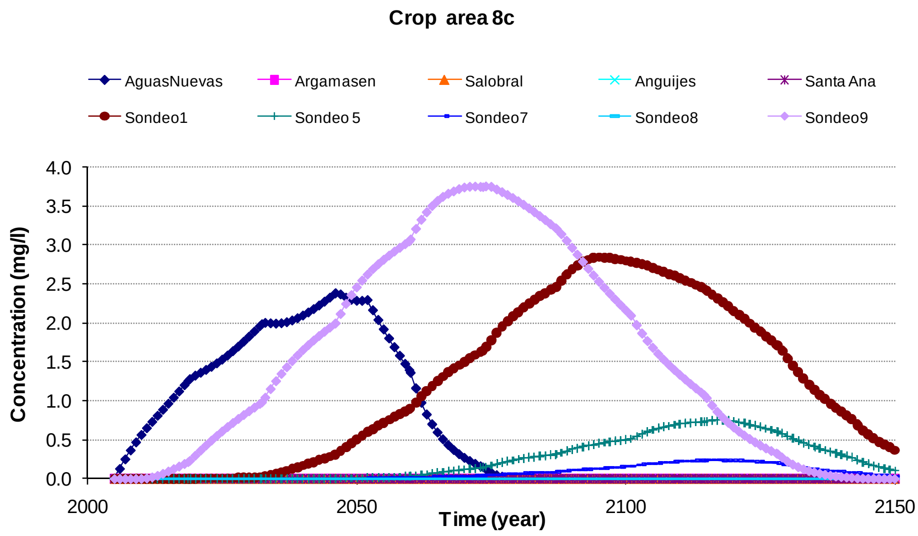


Figure 5.18 Unitary concentration time curves for crop area 8c

The dryland (rainfed crop land) was not taken into account for the management options. However the corresponding nitrate loads were considered. This is done by considering the dryland area is the one of 2005 and a nitrate leaching rate of 20 kg/ha. The influence of the dryland upon the concentration at the observation wells is very low (Figure 5.19).

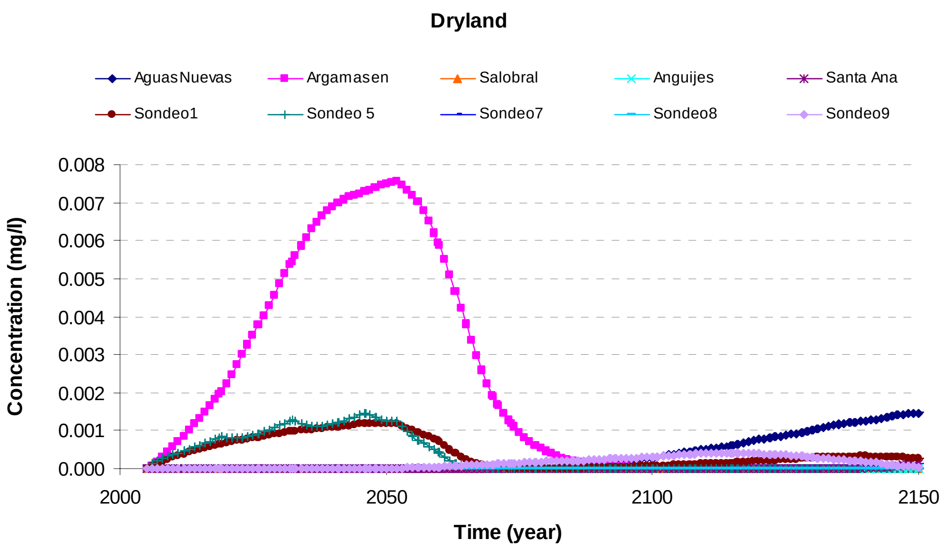


Figure 5.19 Concentration time curves for dry-land

Additional to the dryland, the effect of the initial concentration corresponding to the state of the aquifer in 2005, Figure 5.13) had to be taken into account. The influence at the control sites is shown in Figure 5.20.

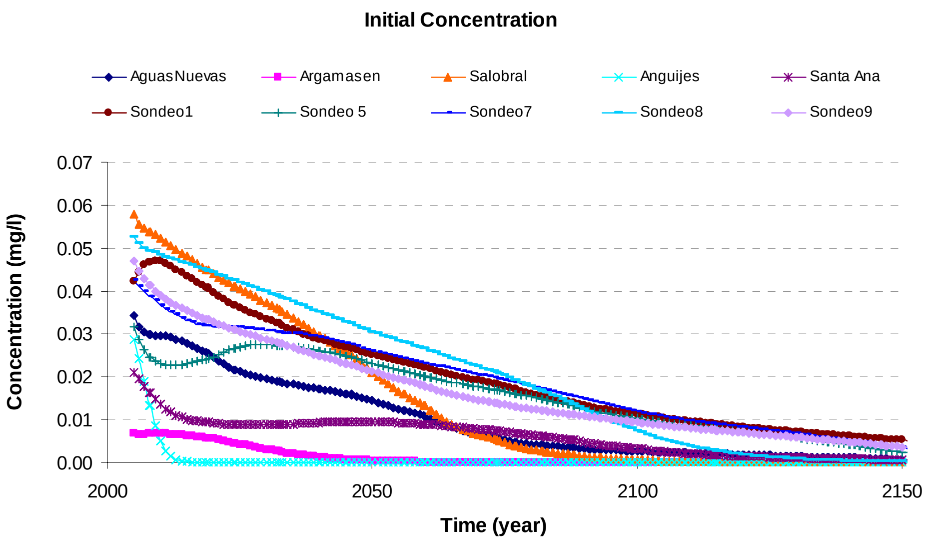


Figure 5.20 Background nitrate concentration derived from the initial nitrate concentration at the control well

The influence of the dryland and the initial concentration were simulated by superposition, modifying equation 4.2 as follows:

$$\sum_{s} RM_{c\times t,s\times y} \cdot cr_{s\times y} + DL_{c\times y} + IC_{c\times y} \leq q_{c\times y} \quad \forall c,t,y$$

(5.1)

where *RM* is the unitary pollutant concentration response matrix; *q* is a matrix of water quality standard imposed at the control sites over the simulation time (kg/m^3); *cr* is a matrix which corresponds to the nitrate concentration recharge (kg/m^3) reaching groundwater from a crop located at source s; *DL* is the nitrate concentration at the control site *c* and the planning horizon *y* due to fertilizer application in dryland and *IC* is the nitrate concentration at the control site *c* and the planning horizon *y* due to the initial nitrate concentrations in the aquifer.

5.5.2 Scenarios

Four scenarios were simulated in order to compare the groundwater nitrate concentrations that could be achieved under different fertilizer management options for the 50 year planning period.

- *Scenario 1. Business-as-usual.* Farmers often over-fertilize crops (e.g. Ramos et al., 2002, in an estimation of N fertilizer use in the Valencia region). This scenario uses the N fertilizer rates that were used to calibrate the nitrate transport model to the observed conditions.
- *Scenario 2. Maximum benefits.* This scenario uses the fertilizer applications that return the maximum net benefits at each crop were used.
- *Scenario 3. Reference values.* The Mancha Oriental System has been declared "nitrate pollution vulnerable area", and maximum values of fertilizer application have been published. This scenario simulates nitrate concentrations under these fertilizer application rates.
- *Scenario 4. Constrained optimal fertilizer application.* This scenario considers the distribution of N fertilizer rates that yields the maximum aggregated net profit constrained to the groundwater nitrate concentration standards (50 mg/l) at the control wells.

The irrigation water applied was kept constant at the level at which the crop yield is maximum (Table 5.9), in order to keep linearity of the problem. The fertilizer and crop prices were taken from the local agronomic institute, ITAP[8]. In this table shows the productions costs that include energy costs, consumables, indirect costs, labor and subsidies. These costs are reported in appendix D.

Table 5.9 Crop, irrigation and prices

Crop	Applied irrigation water [1] (mm/year)	Crop price [1] (€/kg)	Fertilizer price [1] (€/kg)	Production costs [2] (€/ha)	Subsidies [2] (€/ha)
Wheat	260	0.136	0.6	650.8	598.1
Corn	665	0.142	0.6	856.5	424.8
Barley	300	0.115	0.6	604.4	552.0
Alfalfa	900	0.138	0.6	1,051.1	0.0
Onion	650	0.700	0.6	4,204.4	0.0

[1] ITAP, Informacion historica 2005
[2] Ministerio de Medio Ambiente (2005). Costes del agua en la agricultura.

[8] http://www.itap.es/ITAP-LONJA/2precios/Historicos/informacion_historica.asp

5.5.2.1 Scenario 1. Baseline or business-as-usual (BAU) scenario.

This baseline scenario is intended to simulate nitrate concentrations in groundwater if the fertilizer rates of 2005 were maintained, i.e., to show the projected trends in nitrate concentration if the current crop management practices persist. These values are estimated through the calibration of the nitrate transport model. Table 5.10 compares the calibrated fertilizer rates with the fertilizer application rates reported by the local Agronomic Institute (ITAP). We have to consider that farmers often use N inputs higher than the recommended values, and sometimes even greater than what they actually report in the official surveys, as it has been proved using N balances (e.g., Ramos et al., 2002). In any case, the values estimated by calibration are subject to the inevitable uncertainties of the modeling process.

Nitrate leaching values (Table 5.10) are calculated through the nitrate leaching functions reported in section 5.3. The resulting concentrations at the control sites, for the next 50 years are shown in Figure 5.21. This graph tells us that nitrate concentration will continue to increase in the control sites “El Salobral” reaching 72 mg/l and “Sondeo 8” up to 63 mg/l. Both control sites are located under the crop areas 5c and 8o, which are among the biggest sources of nitrate pollution. The nitrate evolution at the control sites “Santa Ana”, “Anguijes” and “Aguas Nuevas” shows an increasing trend, while the others seems to become stable. The WFD sets that good status has to be reached by 2015 by this year the maximum nitrate concentrations (Control site “El Salobral”) would be of about 60 mg/l. Nitrate concentrations at “sondeo 8” will also overpass 55 mg/l. According to these results, the management in the trend scenario would not be “sustainable” (for the EU standards) with regards to nitrate pollution. Regarding the economic results, the net benefits for the period amounts to 96.6 M€/year on average. This result will be later compared with those obtained for the other scenarios to valuate the opportunity cost (considered as benefit forgone) of imposing constraints on groundwater nitrate concentration.

Table 5.10. Fertilizer application and nitrate leaching. Scenario 1

Crop	Actual fertilizer application (kg/ha)[1]	Nitrate leaching (kg/ha)	ITAP Fertilizer application. 2005 (kg/ha)[2]
Corn	315	116	296
Wheat	160	44	144
Barley	165	52	124
Onion	285	94	216
Alfalfa	40	15	20

[1] Values obtained from the calibration of the groundwater nitrate transport model
[2] ITAP (2005). www.itap.es

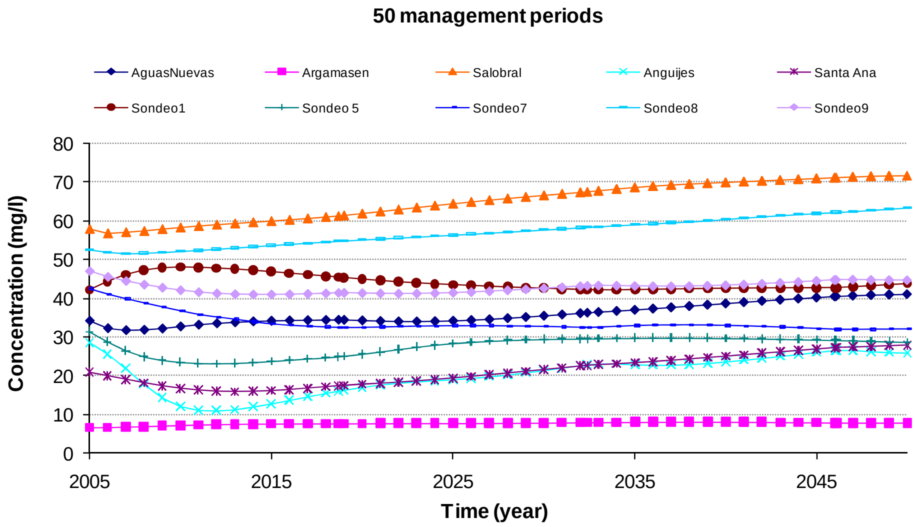


Figure 5.21 Concentration time curves for the current fertilizer application. Scenario 1

5.5.2.2 Scenario 2. Maximum benefits.

In this scenario, the fertilizer application was optimized in order to maximize the total net benefits, without groundwater quality restrictions. The fertilizer loading rates are shown in Table 5.11. These values are lower than the value reported in Table 5.10 referring to the current (calibrated) fertilizer rates (although quite similar for onions and alfalfa). With the required caution given the uncertainties and the lack of data, this tells us that farmers might be over-fertilizing their crops, which is in agreement with the finding of other authors (e.g., Ramos et al., 2002). With these applications the total net benefits amounts to 96.7 M€/year (quite close to the average values obtained in the BAU scenario). The maximum concentration goes up to 66.7 mg/l in *"El Salobral"* control site (Figure 5.22). The nitrate concentration in the control sites exhibits a very similar trend than in scenario 1, but with slightly lower values since less fertilizer is applied. Even though the nitrate concentrations are lower, the water quality objectives are not met making this scenario unsustainable for the EU environmental standards.

Table 5.11. Fertilizer application and nitrate leaching. Scenario 2

Crop	Maximum benefit fertilizer application (kg/ha)	Nitrate leaching (kg/ha)
Corn	283	105
Wheat	141	38
Barley	146	46
Onion	282	93
Alfalfa	39	14

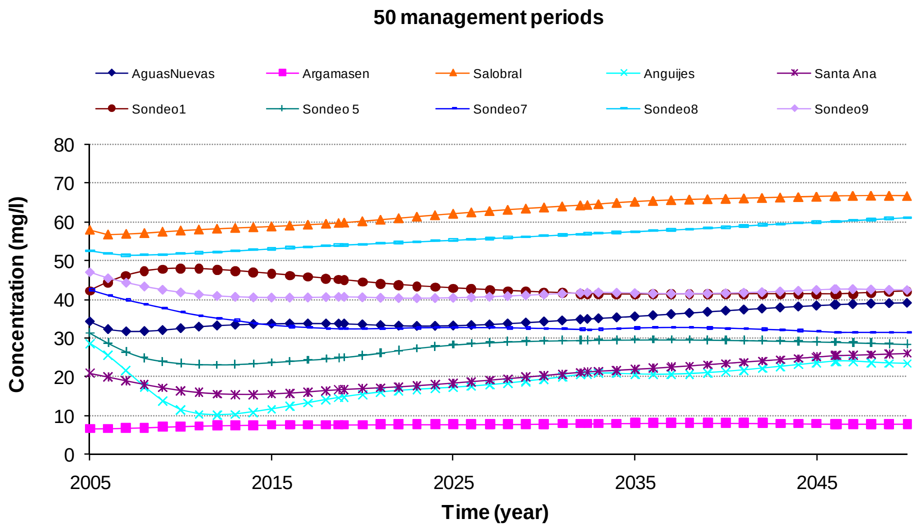


Figure 5.22 Concentration time curves for the fertilizer application that yields the maximum benefits. Scenario 2

5.5.2.3 Scenario 3. Reference values.

The Mancha Oriental System has been defined as "nitrate pollution vulnerable area" in the DOCM *"Diario Oficial de Castilla La Mancha"* (DOCM, num 16 January 22nd, 2007). The maximum nitrogen fertilizer reported is (Table 5.12):

Table 5.12. Reference values for maximum nitrate fertilizer application (kg/ha) (DOCM, 2007)

Crop	Fertilizer application (kg/ha)
DryLand	
Barley	60
Wheat	70
Irrigation	
Barley	110
Corn	210
Wheat	110
Alfalfa	35
Onion	160

The maximum nitrate concentrations obtained with the reference values are shown in Figure 5.23. Even though the maximum nitrate concentrations are above 50 mg/l in the control sites "El Salobral" and "Sondeo 8", given the high starting conditions they do not show an increasing trend. However, in order to reduce nitrate concentration below the 50 mg/l more reduction of fertilizer application would be necessary. For this scenario the net benefits average are 80.9 M€/year, a 16% less than the average net benefits for the BAU scenario.

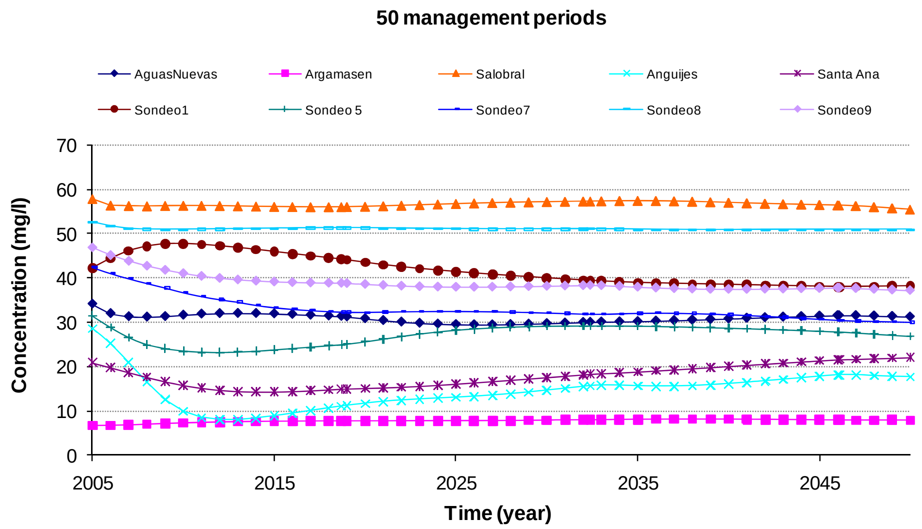


Figure 5.23 Concentration time curves for the maximum allowed fertilizer application. Scenario 3

5.5.2.4 Scenario 4. Constrained optimal fertilizer application

This scenario is intended to determine the optimal spatial distribution of fertilizer application over 50 years of planning horizon that meets the groundwater nitrate concentration limits by two time horizons: year 2015 (first deadline for the achievement of environmental objectives in the EU WFD) and year 2021 (which correspond to the second deadline, 6 years later) . To consider possible long-term effects of the 50 years of fertilizer application, nitrate transport in groundwater is simulated for more than 100 years. In the following figures the results are shown only until year 2055, since after this year no more fertilizer is applied and the nitrate concentrations decay after.

Recovery time 2015

Table 5.13 shows the results of the optimization referring to fertilizer application, reduction from actual use (Scenario 1, BAU) and profits, for the case in which groundwater nitrate concentrations below 50 mg/l are imposed beyond year 2015. Figure 5.24 depicts the spatial allocation of the fertilizer reductions. 5c and 9c are the areas that need the biggest reduction. The area 5c has a big influence on the concentration of the control site *"El Salobral"*, as 9c has on the control site *"Sondeo 8"*, the one in which the highest concentrations are reached. 40 kg/ha is very low rate for corn, making this crop not very attractive for farmers. The total profits are 95.4 M€/year, only a 1.2% lower then scenario 1 (96.6 M€/year).

The nitrate concentrations at the control sites that results from applying the fertilizer shown in Table 5.13 are depicted in Figure 5.25. The maximum values are below 50 mg/l. Note that the maximum concentrations are observed in control site *"Sondeo 8"*.

The results obtained by superposition were compared with the ones obtained simulating the optimal fertilizer application with MT3DMS (Zheng and Wang, 1999), the mass transport code that was used for assembling the concentration response matrix. The results for the control sites with higher concentrations are shown in

Figure 5.26. As can be seen, the values from both simulations are very close, showing that the assumption of linearity and consequently the steady-state flow conditions (see section 4.1.1) has not a big influence upon the results.

Table 5.13 Optimal fertilizer application. Recovery time 2015

Crop	Area	Fertilizer application (kg/ha)	Nitrate leaching (kg/ha)	Fertilizer reduction (%)	Profit (€/ha)
Barley	1b	146.0	46	12%	571
Wheat	1w	141.2	38	12%	742
Alfalfa	2a	36.9	14	8%	1,017
Corn	2c	283.3	105	10%	1,341
Wheat	2w	141.2	38	12%	742
Corn	3c	283.3	105	10%	1,341
Wheat	3w	141.2	38	12%	742
Corn	4c	283.3	105	10%	1,341
Corn	5c	39.7	20	**87%**	785
Corn	6c	283.3	105	10%	1,341
Corn	7c	283.3	105	10%	1,341
Onion	7o	281.8	93	1%	46,557
Alfalfa	8a	36.9	14	8%	1,017
Corn	8c	283.3	105	10%	1,341
Onion	8o	281.4	93	1%	46,557
Corn	9c	119.6	47	**62%**	1,090
Onion	9o	281.8	93	1%	46,557
Wheat	9w	141.2	38	12%	742
Barley	10b	146.0	46	12%	571
Corn	10c	283.3	105	10%	1,341
Wheat	10w	141.2	38	12%	742
Corn	11c	283.3	105	10%	1,341
Corn	12c	283.3	105	10%	1,341

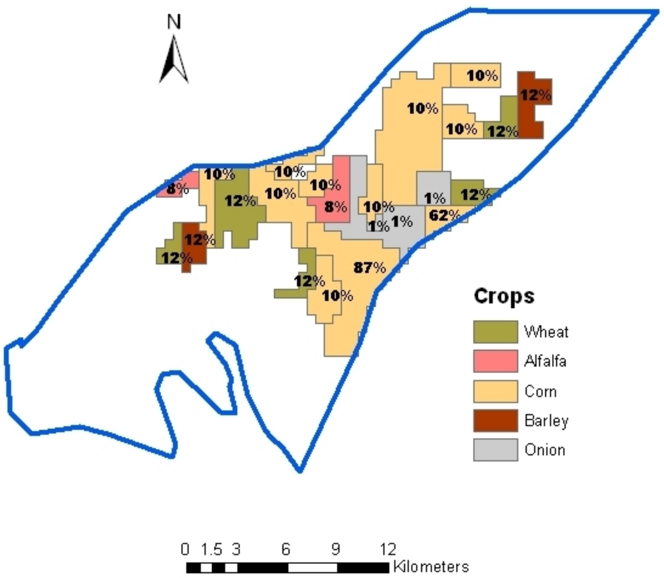


Figure 5.24 Allocation of fertilizer reduction. Recovery time 2015

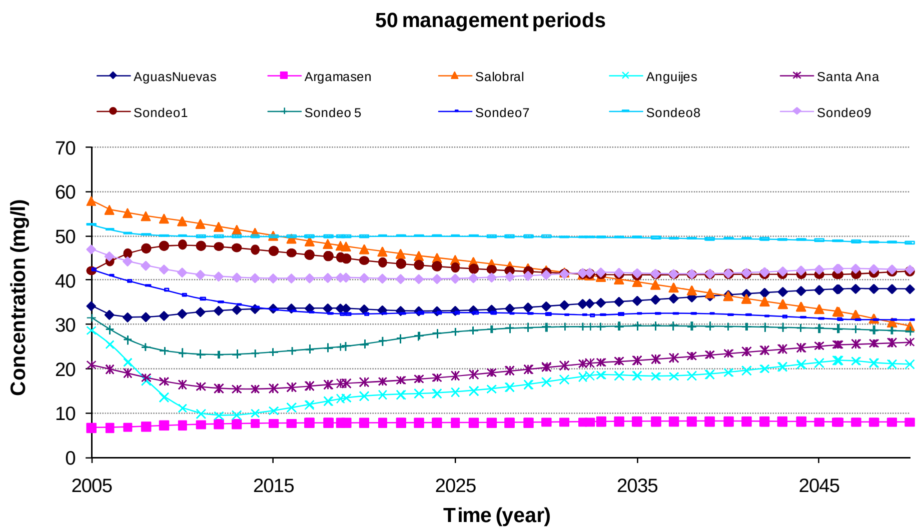


Figure 5.25 Concentration time curves for the optimal fertilizer application. Recovery time 2015

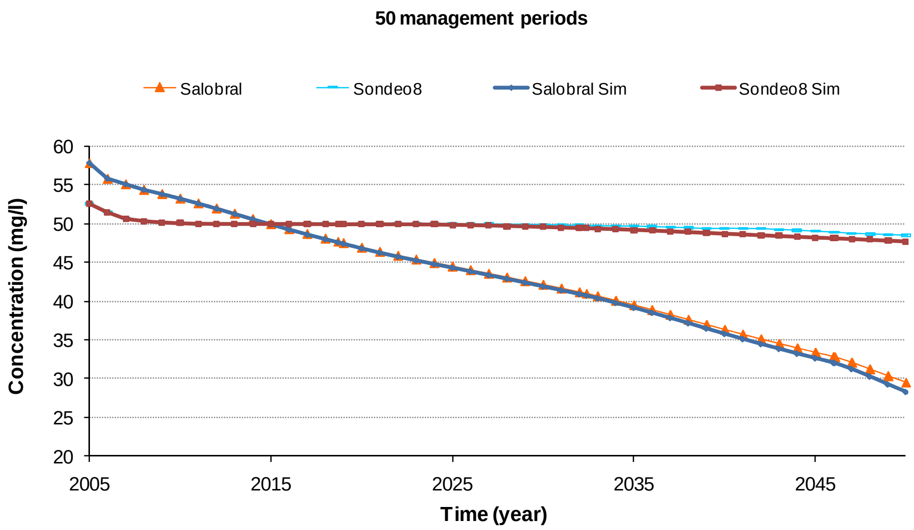


Figure 5.26 Concentration time curves by superposition vs simulated. Recovery time 2015

Recovery time 2021

An additional simulation was performed to obtain the optimal fertilizer application considering that the quality standards had to be met in 2021 and instead of 2015. This could be useful for an analysis of derogations in the application of the WFD, according to the considerations of article 4 of the Directive. The results show that in this case the fertilizer application in area 5c had to be reduce to a 68% of the current application (103 kg/ha) (Table 5.14). The average total net benefits were of 96.0 M€/year are higher than in the scenario of recovery fro 2015 (95.4 M€/year), as expected. The allocation of the fertilizer reduction is presented in Figure 5.27. Figure 5.28 shows the resulting nitrate concentrations at the control sites. When the recovery time is increased, the fertilizer reduction in area 5c becomes lower; nitrate concentrations in the control site *"El Salobral"* are below 50 mg/l after year 2021.

Table 5.14 Optimal fertilizer application. Recovery time 2021

Crop	**Area**	**Fertilizer application (kg/ha)**	**Nitrate leaching (kg/ha)**	**Fertilizer reduction (%)**	**Profit (€/ha)**
Barley	1b	146.0	46	12%	570.8
Wheat	1w	141.2	38	12%	741.6
Alfalfa	2a	36.9	14	8%	1017.0
Corn	2c	283.3	105	10%	1341.2
Wheat	2w	141.2	38	12%	741.6
Corn	3c	283.3	105	10%	1341.2
Wheat	3w	141.2	38	12%	741.6
Corn	4c	283.3	105	10%	1341.2
Corn	5c	101.8	41	**68%**	1032.3
Corn	6c	283.3	105	10%	1341.2
Corn	7c	283.3	105	10%	1341.2
Onion	7o	281.8	93	1%	46556.8
Alfalfa	8a	36.9	14	8%	1017.0
Corn	8c	283.3	105	10%	1341.2
Onion	8o	281.0	93	1%	46556.4
Corn	9c	117.1	47	**63%**	1082.1
Onion	9o	281.8	93	1%	46556.8
Wheat	9w	141.2	38	12%	741.6
Barley	10b	146.0	46	12%	570.8
Corn	10c	283.3	105	10%	1341.2
Wheat	10w	141.2	38	12%	741.6
Corn	11c	283.3	105	10%	1341.2
Corn	12c	283.3	105	10%	1341.2

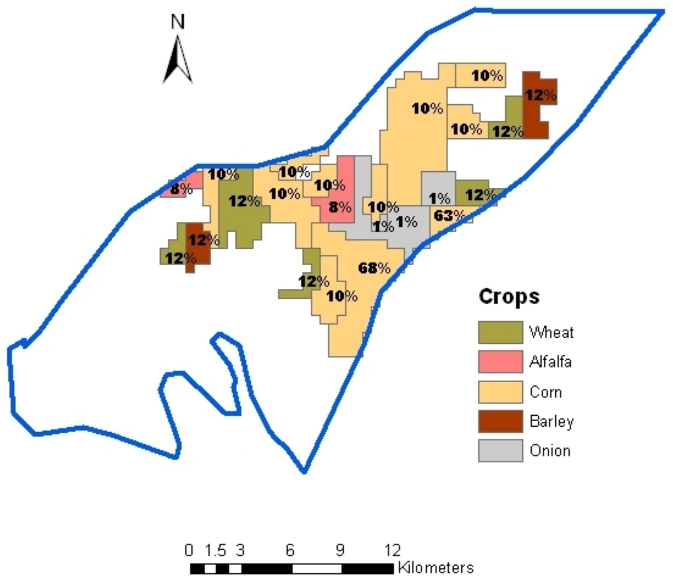


Figure 5.27 Allocation of fertilizer reduction. Recovery time 2021

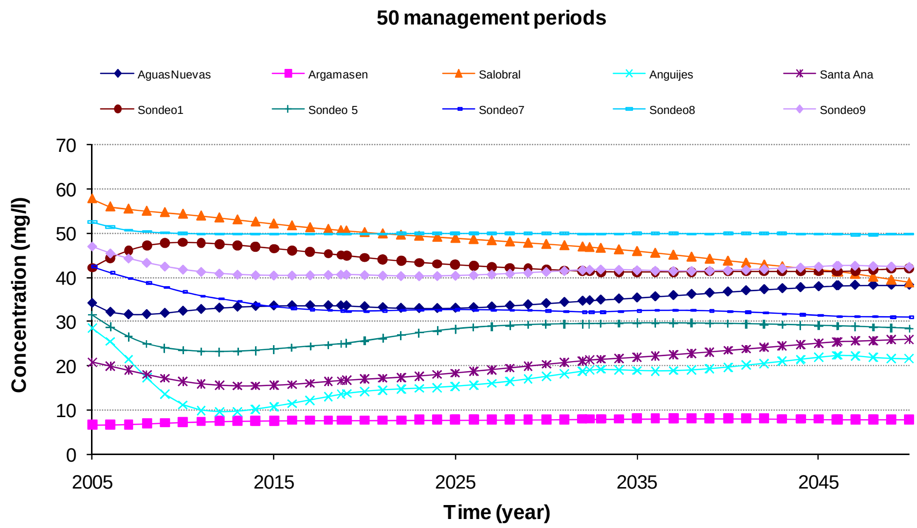


Figure 5.28 Concentration time curves for the optimal fertilizer application. 2021

Table 5.15 shows a comparison between the different scenarios. The BAU scenario (scenario 1) leads to the highest nitrate concentrations, reaching values of 71.7 mg/l but it returns an average net benefits of 96.6 M€/year. This value is very close to the maximum net benefit scenario (scenario 2) of 96.7 M€/year, although the nitrate concentrations in the scenario 2 are lower (lower fertilizer applications). In spite of using more fertilizer in scenario 1 than 2 the resulting net benefits are lower, since the costs are higher and no grater crop yield is obtained out of that fertilizer excess.

Applying the fertilizer rate recommended for nitrate vulnerable zones in *"La Mancha"* (DOCM, 2007) (scenario 3), the maximum nitrate concentrations in groundwater becomes 57.5 mg/l, much lower than in BAU scenario. In fact, the maximum nitrate concentrations are mostly inherited from the high initial concentrations and not because of the fertilizer use after 2005. However, in this scenario the total net benefits are reduced by 15.7 M€/year, and it still does not comply with the 50mg/l standard. This implies that applying the Nitrate Directive in not an optimal option.

In scenario 4 for 2015 recovery time, the total net benefits are 95.4 M€/year, just 1.2 M€/year lower than the maximum net benefits scenario, and 15.5 M€/year more than in the scenario 3. This 1.2 M€/year would be the estimate of the cost (in terms of net benefits forgone) of complying with the WFD in relation to groundwater nitrate pollution for year 2015. For the planning period of 50 years, this amounts to 60 M€. If the quality standard is imposed in year 2021, the cost of compliment would be reduced to 30 M€. In order to justify derogation as permitted by article 4 of the WFD, the cost of reaching the objective in 2015 and not in 2021 should be compared with the avoided treatment cost for drinking water utilities.

Table 5.15. Comparison among scenarios.

	Average fertilizer application (kg/ha)	**Maximum nitrate concentration (mg/l)**	**Total net benefits (M€/year)**
Scenario 1. Business as usual	240.4	71.7	96.6
Scenario 2. Maximum benefits	218.7	66.7	96.7
Scenario 3. Reference values	157.8	57.5	80.9
Scenario 4. Optimal fertilizer. 2015	201.1	50.0 (after 2015)	95.4
Scenario 4. Optimal fertilizer. 2021	203.7	50.0 (after 2021)	96.0

Figure 5.29 and Figure 5.30 show nitrate concentration at the most critical control sites, *"El Salorbal"* and *"Sondeo 8",* for the different scenarios. The only scenario in which nitrate concentrations are reduced below the target is scenario 4. For the control site *"Sondeo 8"* nitrate concentrations are reduced below 50 mg/l and maintained very close to that value in the whole planning period, while nitrate concentration in the control site *"El Salorbal"* are steadily dropping. If the optimal fertilizer application were allowed to vary over the planning horizon, nitrate concentrations could be maintained close to 50 mg/l during the whole simulated period.

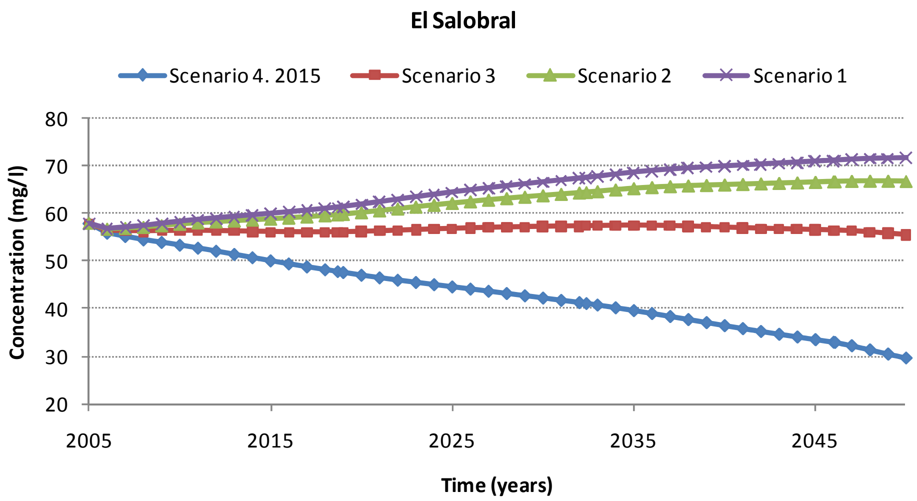


Figure 5.29. Concentration time curves for different scenarios at control site *"El Salobral"*.

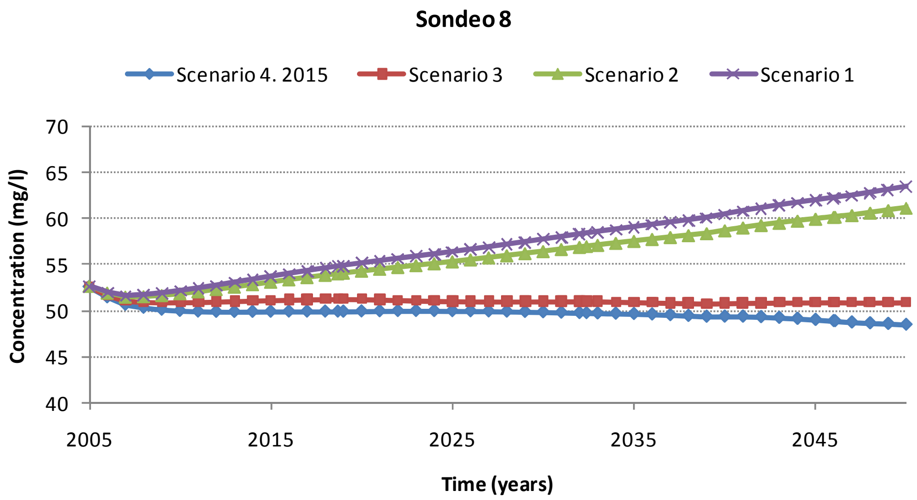


Figure 5.30. Concentration time curves for different scenarios at control site *"Sondeo 8"*.

"El Salorbal" and *"Sondeo 8"* are the control sites most affected by pollution, and the crop areas 5c and 9c are the polluters with bigger influence over them. Another simulation was performed to limiting the percentage of fertilizer reduction in these areas, but the problem turned out to be infeasible, since the other crop areas have very little influence over these control sites.

5.6 Fertilizer tax

The results of applying fertilizer standards (according to the optimal values reported for scenario 4 discussed above) were compared with the ones obtained using taxes on fertilizer. Several optimizations were carried out in order to obtain the fertilizer tax that would reduce its use to the level were the nitrate leached does not generate nitrate concentrations in groundwater above 50 mg/l. For this, the fertilizer price in the optimization model was parameterized, increasing its value until the nitrate concentration sin groundwater was below 50 mg/l.

In order to reach nitrate concentrations below 50 mg/l in all control sites, the fertilizer price has to be increased up to 5.15 €/kg (i.e., a tax of 858 % would be required); in that case the profits will go down to 86.6 M€/year. Figure 5.31 shows the results of these simulations. The benefits obtained by increasing the fertilizer price are 8.9 M€/year lower than those obtained from the fertilizer standards corresponding to scenario 4.

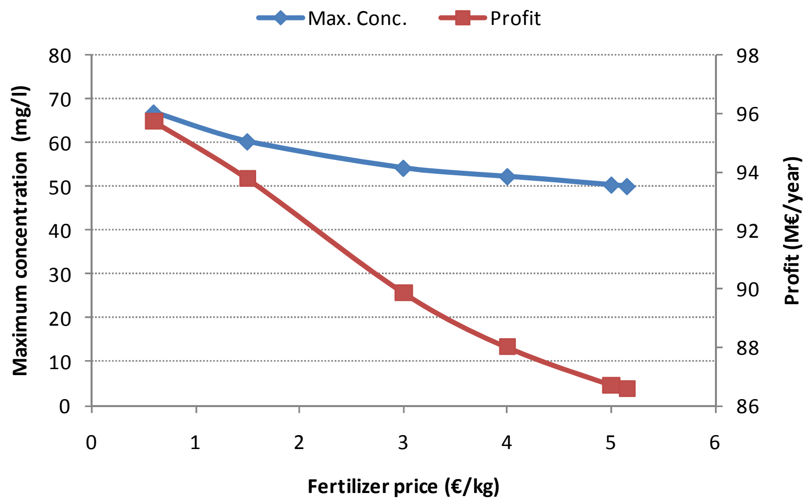


Figure 5.31 Maximum nitrate concentration achieved with different fertilizer price and total benefits

These results suggest that farmers are not sensitive to fertilizer tax until it reaches a very high level. However, we have to keep in mind that this model assumes that farmers only adjust the level of fertilizer use but not change crops. In reality farmers may decide to stop producing one crop or switch to another one, in response to changes in prices.

Discussion

This chapter showed the application of the method to a real application case that faces problems of increasing nitrate concentration in certain zones. . The results obtained for the BAU or baseline scenario (scenario 1) show that following the current fertilizer application rates does not guarantee to comply with the "good groundwater chemical status" required by the WFD, since the standard of 50 mg/l of nitrates would be overpassed.). The fertilizer application that generates the maximum net benefits (scenario 2) are lower than those obtained by calibration of the nitrate transport model in order to reproduce the observed nitrate concentrations in scenario 1 (which are also a bit higher than those reported in the official surveys). The reference values requested by the authorities because of the definition as "nitrate vulnerable zone" maintain groundwater nitrate concentrations stable; however, the maximum nitrate concentrations are still over 50 mg/l, since the initial values (year 2005 concentrations) were already above the target value. The total net benefits of this scenario is lower than for the scenario 4 (optimal fertilizer application constrained by the quality standards) because the reduction was applied to all crops without taking into consideration the influence of the spatial distribution of the crops upon nitrate concentrations in the control sites. The scenario 4 showed the fertilizer application rates that will yield the maximum total net benefit while complying with the quality standards for two different horizons: year 2015 and year 2021. Therefore, these values can be interpreted as the “fertilizer standards” that should be imposed in order to meet the standards at the least cost. Even though the policy of fertilizer standards has appeared as more cost-efficient, in real applications it can be difficult to implement and to control. Fertilizer taxes are a promising option, being easier to apply and control. Some countries are now discussing its practical implementation. For example, the Swedish Environmental Protection Agency has proposed the use of a permit fee system for nitrogen and phosphorus with the aim of reducing nitrogen and phosphorus loads to the Baltic Sea and the West Sea (SEPA, 2009). The proposal entails setting a cap for discharges for example from agriculture, sewage treatment plants and industrial plants. Anyone wishing to discharge more than the cap has to pay a fee which funds an equivalent reduction in discharges elsewhere. It can also be possible to sell and buy discharge credits in the fee market.

6 Stochastic modeling framework

One of the most difficult issues in groundwater management modeling is dealing adequately with the effect of model uncertainty in optimal decision making (Wagner and Gorelick, 1987). The uncertainty stems from a wide variety of factors ranging from partial knowledge about the aquifer properties, its boundary conditions, land use practices, on-ground nitrogen loading, nitrogen soil dynamics, soil characteristics, depth to water table, flow and transport parameters affecting nitrate fate and transport in groundwater, to economic, regulatory and political factors.

6.1 Stochastic modeling framework

The heterogeneity of hydraulic conductivity field has a strong influence on the migration and evolution in time and space of the pollutant concentration in groundwater. The hydraulic conductivity of an aquifer can vary spatially by several orders of magnitude. Given the uncertainty in the conductivity, our groundwater flow and mass transport predictions, based on the conductivity fields, will be uncertain. Therefore, the uncertainty of the K spatial variability should be incorporated into the decision process in order to derive an optimal strategy to control groundwater nitrate pollution with certain reliability.

The main goal of this chapter is to analyze the influence of uncertainty in the physical parameters of a heterogeneous groundwater diffuse pollution problem on the results of management strategies, and to introduce methods that integrate uncertainty and reliability in order to obtain strategies of spatial allocation of fertilizer use in agriculture. A systematic stochastic framework is presented using four different formulations, to explicitly incorporate the effects of uncertainty through to the design of reliable groundwater quality schemes. The stochastic approaches for dealing with uncertainty require the generation of multiple realizations of K fields, which can be obtained by means of any geostatistical approach existing in the literature such as interpolation methods, sequential Gaussian or indicator simulation, conditional K fields obtained from inverse models, etc. Obviously, the uncertainty in the results will be strongly influenced by the variance of the hydraulic conductivity probability distribution and the spatial correlation structure. Therefore, the aquifer should be characterized as adequately as possible in order to obtain reliable results. Moreover, a sensitivity analysis with regard the uncertain parameters should accompany a work like this.

6.1.1 Monte Carlo simulation with pre-assumed ("true") parameter field

The objective is to evaluate the reliability of the optimal fertilizer application for an aquifer with a pre-assumed heterogeneous hydraulic conductivity field. This is carried out by assuming one of the multiple K fields generated as the "true" hydraulic conductivity field (e.g., Bakr et al., 2003; Ko and Lee, 2008). Subsequently, the corresponding optimal fertilizer application is obtained by using the deterministic formulation presented above (hereinafter, it will be called the pre-assumed optimal fertilizer application). However, because this K field is not necessarily true, the pre-assumed optimal fertilization scheme could succeed or fail the maximum concentrations allowed when applied to the different K fields by means of Monte Carlo simulations. Therefore, the reliability level and the uncertainty of the pre-assumed optimal application are evaluated by applying the designs to each of the random fields generated stochastically, and tested as to whether the maximum concentrations were reached or not.

6.1.2 Monte Carlo optimization

Monte Carlo management models solve the nonlinear simulation-optimization problem individually for a single scenario representing uncertainty. Because of its simplicity a lot of works in the literature have pointed out towards this formulation to assess the uncertainty (e.g., Gorelick 1983; Wagner and Gorelick, 1989; Freeze and Gorelick 1999; Thorsen et al., 2001; Mayer et al. 2002; De Vries et al., 2003; Kroeze et al., 2003; Feyen and Goelick, 2004; Lacroix et al., 2005; Ko and Lee, 2008; Van den Brink et al., 2008). Therefore, in this formulation a series of individual optimization problems are solved, each with a single realization of hydraulic conductivity. In order to account for the uncertainty associated with the heterogeneous K fields the hydro-economic modeling is solved for each realization, i.e., the optimization problem presented in equations (4.1)-(4.2) is solved for each realization individually. Thereby, if there are *i* hydraulic conductivity fields, the Monte Carlo management model will provide *i* optimal fertilizer applications, each one corresponding to a different realization of hydraulic conductivity.

Since the K field is assumed to be random, the optimal fertilizer application is also random. Each of the *i* fertilizer applications obtained from the hydro-economic model represents a random sampling from the cumulative density function (CDF) of optimal fertilizer application rates. Therefore the results of the Monte Carlo hydro-economic modeling can be used to characterize the probability distribution of the optimal fertilizer application rates.

6.1.3 Multiple realizations or stacking management model

Multiple realization or stacking management model simultaneously solve the nonlinear simulation-optimization problem for a set of different scenarios representing uncertainty, e.g., by using a sampling of hydraulic conductivity realizations generated using geostatistical techniques (Wagner and Gorelick, 1989; Aly and Peralta, 1999; Feyen and Gorelick, 2004; Feyen and Gorelick, 2005; Ko and Lee, 2009). However, this approach does not allow a priori definition of the desired system reliability. The reliability is determined through post-optimization Monte Carlo analysis on a much larger set of realizations that were used in the stack. Since the reliability of the system management is not explicitly considered in the optimal solution, the method can lead to conservative (and more expensive) solutions, although some authors have pointed out that based on a few number of scenarios this approach can provide reliable (over 90%) groundwater quality strategies (e.g.,Wagner and Gorelick, 1989).

The mathematical formulation of the multiple realization groundwater quality management model consist of maximize (4.1) subject to:

$$\sum_{s} RM_{(c\times t, s\times y)_i} \cdot cr_{(s\times y)_i} \leq q_{(c\times t)} \quad \forall i, c, t, y \tag{6.1}$$

where an additional component *i* is added to the response matrix considered in the deterministic hydro-economic management model. This component is made up with as many elements as realizations of the random conductivity field are simultaneously considered in the management model. That is, the optimization problem is solved for $i = 1, \ldots, s_n$, where *i* represents a hydraulic conductivity realization; and s_n is the stack size, which is the number of hydraulic conductivity realizations included in the stochastic management model. The optimization problem retains the same number of decision variables as the deterministic model, but the number of concentration constraints is increased by a factor of *i*. Thereby, the concentration constraints must be satisfied for each one of the conductivity fields, and the optimal fertilizer application would be feasible for any of the optimization sub-problems. It is guaranteed to be successful for each *i* different realizations. The reliability is determined through post-optimization Monte Carlo analysis on a much larger set of realizations that were used in the stack.

6.1.4 Mixed-integer stochastic optimization model with predefined reliability

Morgan et al. (1993) introduced a mixed-integer approach to solve an optimization model to find an optimal remediation design with certain reliability. The approach combines the advantages of the simulation-optimization models with those of the chance-constrained models. In this case, the user selects the desired degree of reliability, which is accomplished by allowing a certain number of the Monte Carlo realizations to fail. Other authors have applied this technique, which has also been termed as mixed-integer-chance-constrained programming (MICCP), e.g., Ritzel et al. (1994), Dhar and Datta (2007), and Ng and Eheart (2008).

We have reformulated the approach presented by Morgan et al. (1993) to deal with nitrate pollution abatement, meeting certain groundwater quality standards, as the ones ruled by the EU Water Framework Directive. The proposed stochastic management problem was defined as the optimal fertilizer allocation that maximizes the welfare from crop production subjected to certain stochastic environmental constraints.

The chance-constrained problem is reformulated as a Mixed Integer Non Linear Programming (MINLP). As in Morgan et al. (1993), the stochastic nature of the conductivity field is analyzed through Monte Carlo realizations, and multiple realizations make up constraint sets of the optimization model (in this case, represented by pollutant concentration response matrices, as in Peña-Haro et al., 2009). The desired reliability of the system is predetermined by fixing the number of constraints that may be violated, which is done by replacing equation (4.1) with equations (6.2) to (6.5). The stochastic method is formulated as follows:

$$Max \prod = \sum_{s}\sum_{y}\frac{1}{(1+r)^{y}} A_s\left(p_s \cdot Y_{s,y} - p_n \cdot N_{s,y} - p_w \cdot W_{s,y} - C_s + S_s\right) - M \cdot \sum_{i} F_i \tag{6.2}$$

subject to:

$$\sum RM_{(c\times t, s\times y)_i} \cdot cr_{(s\times y)_i} - M \cdot f_{(c\times t)_i} \le q_{(c\times t)_i} \quad \forall i, c, t, y \tag{6.3}$$

$$\sum_{c,t} f_{(c \times t)_i} \leq M \cdot F_i \quad \forall i$$

(6.4)

$$\sum_{i} F_i \geq NF \quad i = 1, \ldots, NR$$

(6.5)

where *M* is a large positive number; *i* is the hydraulic conductivity realization number, *NR* is the total number of realizations; *f* is a matrix with binary values made of four components, where *i* is the realization number, *c* refers to control site, *t* stands for simulated time step, and *y* is the planning year. The matrix represents the individual failures, and its components take the value 1 if the quality standard is exceeded at any time in any control site, and 0 otherwise; *F* is a binary vector with *i* elements showing realization failures. It takes the value 1, thus representing a failure, if the quality standard is exceeded in at least one time step at any control site for a certain realization *i*, and 0 otherwise. *NF* is the number of realization failures that are allowed, defined in accordance with the desired reliability level, *R*, which is given by,

$$R = 1 - \frac{\sum_{i} F_i}{NR}$$

(6.6)

Therefore, reliability is maintained by constraining the number of failures allowed. Note that with this formulation for each realization *i*, a failure (F_i=1) is considered when the quality standard is not met, independently on how many times or in how many control sites the quality standard is exceeded. Therefore, for a single realization *i*, *f* may exceed the quality standard in several times steps or control sites, thus leading to define F_i as a failure, i.e., F_i =1. Finally, failures are penalized in the objective.

Unlike the classic chance-constrained applications (e.g., Tung, 1986; Wagner and Gorelick 1987; McSweeny and Shortle, 1990; Wagner 1999), this formulation considers uncertainty in the response matrix coefficients and does not require a priori definition of the distribution. The "classic" chance-constrained programming (Charnes et al., 1958; Charnes and Cooper, 1963) is a stochastic programming method that enables the integration of parameter uncertainties into the optimization framework at time that permits constraint violations up to specified probability limits. Therefore, this technique allows tackling problems where some or all parameters are described by random variables, and allows the determination of optimal groundwater quality management subject to a specified system performance reliability requirement. The general chance-constrained method is defined as:

Optimize f(c,x)

subject to: $Pr\ (Ax \leq b) \geq R$

where P_r means probability; x is a n vector of decision variables; A, b and c may contain random variables and represent respectively, *a* m × n matrix, *m* and *n* vectors of parameters; and R is a m vector of desired reliability levels.

This problem has been usually solved in the literature by transforming the probabilistic constraints to deterministic equivalents given knowledge of the distribution function, which simplify the problem in order to transfer the randomness to the right-hand side of the constraint. The deterministic equivalent-based methods can be solved by linear or nonlinear programming methods (e.g., Charnes and Cooper, 1963; Kataoka, 1963). Nevertheless, they entail a series of drawbacks such as requiring assumptions of parameter distributions that may induce to errors (for mathematical convenience, the most widely used statistical model is the normal distribution, e.g., Tung, 1986; Wagner and Gorelick, 1987), or to be unsuitable for complex nonlinear problems where the deterministic equivalent may be difficult or even impossible to establish. Furthermore, they become cumbersome whenever reliability is defined as the probability of meeting a set of constraints simultaneously, rather than one or more (Ng and Eheart, 2008). All these problems are avoided with the approach here presented. However, the chance-constrained approach has also the advantage of requiring less computational effort that the multiple realization model or the mixed-integer models.

6.2 Synthetic case study

In order to illustrate the application of the stochastic management model, the formulations described was applied to a synthetic case study with the same geometry and external stresses than the one presented in chapter 4, with the difference that in this case the K field is not homogenous.

A 40 year planning horizon was considered for each scenario, with a constant annual fertilizer application during the 40 years. . All the optimization models are coded in GAMS (GAMS, 2008). The nonlinear optimization models were solved using CONOPT (Drud, 1985), which is based on the Generalized Reduced Gradient algorithm designed for large programming problems. The optimization problem reformulated as a MINLP iThe aquifer system configuration is the same that the used in section 5.2, which apply the deterministic formulation to a 2D synthetic aquifer with a homogeneous hydraulic conductivity of 40 m/day. In this case, however, we consider heterogeneous hydraulic conductivity.

The aquifer has impermeable lateral boundaries and steady-state flow with direction top to bottom of Figure 4.4. The finite difference grid is 30x41 km with a grid size of 500 x 500 meters. A confined aquifer has been modeled with a thickness of 10 meters, effective porosity of 0.2, and longitudinal dispersivity of 10 meters and a transversal dispersivity of 1 meter. The natural recharge is 500 m^3/ha. There are 70 stress periods, each of one year (365 days). Seven different crop zones (pollution sources or just sources in our model formulation) 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 4.4. Three control sites with concentration upper bounds of 50 mg/l of nitrates, as established by the EU water legislation, are imposed.

6.2.1 Simulation of conductivity fields

The different stochastic optimization management formulations require the generation of multiple K fields. The simulation of these K fields, in the 2D synthetic case stated above, has been performed by means of a sequential Gaussian simulation using the computer code GCOSIM3D (Gómez-Hernández and Journel, 1993). The stochastic structure is assumed to be common for all simulated K fields; thus we simplify our analysis avoiding the uncertainty on the stochastic structure. Therefore, all K fields are equally likely realizations, and therefore, are plausible representations of reality.

The stochastic structure has been defined by using a spherical variogram with a range approximately equal to 1/5 of the aquifer size, 0.5 of nugget effect, and sill of 4. The effect of different degrees of heterogeneity of the parameters in the aquifer has been studied. Specifically, a sensitivity analysis by considering two different variances of the hydraulic conductivity distribution has been carried out, both with a normal distribution with mean 40 m/day and with variances of 15 m^2/day^2 (referred as “case 1”) and 60 m^2/day^2 (“case 2”). A hundred realizations were generated for each case. We assume that this set is large enough to provide a significant representation of the variability of the parameter. Figure 6.1 illustrates the K field for the realization #1, while Figure 6.2 shows the frequency distribution and univariate statistics for all K realizations.

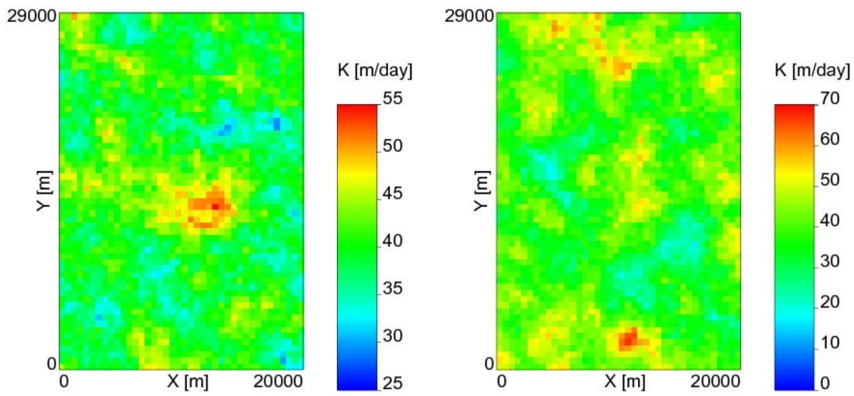


Figure 6.1 *K* field for realization #1 and variances of 15 (left) and 60 (right)

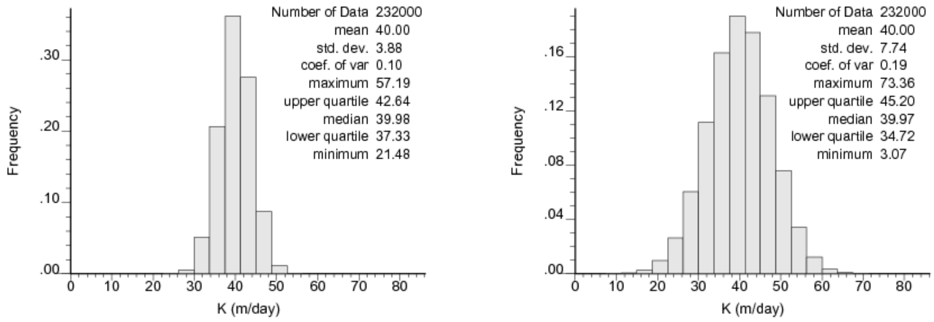


Figure 6.2 Frequency distribution and univariate statistics for all K realizations and variances of 15 (left) and 60 (right).

6.2.2 Pollutant concentration response matrices

Once the different conductivity fields were generated, the pollutant concentration response matrices were ensembled. The pollutant response matrix describes the influence of pollutant sources upon concentrations at the control sites over time. 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. To construct the pollutant concentration response matrix the flow and transport governing equations must be solved. MODFLOW (McDonald and Harbough, 1988), a finite difference groundwater flow model, and MT3DMS (Zheng and Wang, 1999), a solute transport model were used. For each K field realization a unitary pollutant concentration response matrix was generated. Therefore, a hundred pollutant response matrices are generated. For this, it was simulated 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.

6.2.3 Monte Carlo simulation with pre-assumed ("true") parameter field

For this case, we have chosen one of the realizations (realization 14) as the "true" K field The resulting optimal fertilizer application is then tested on the random fields generated to check the reliability of meeting the water quality standard (Monte Carlo simulation). Figure 6.3 shows the reliability or probability of not exceeding certain nitrate concentration level for the two cases with different variances, obtained from the maximum concentration values simulated at each conductivity field for the optimal fertilizer application of the "true" parameter field. The reliability level of the pre-assumed optimal policy for meeting the quality standard was only a 24% for the case 2, i.e., only in 24 realizations out of the 100 simulated nitrate concentrations do not exceed the limit of 50 mg/l. With a bigger variance, although the reliability of meeting the standard is higher (24% against 14%), the range of possible maximum concentrations increases, which can be an important issue in the design of risk-averse policies.

Reducing the obtained fertilizer application rate, we can increase the reliability level to 100%. We have estimated that, for case 2, the mean application rate has to be reduced by 20% to obtain a global reliability of 100% when checked with the 100 realizations. This result was obtained by lowering the constraining quality standard (to 30.6 mg/l), as proposed by Ko and Lee (2008) for the analysis of the optimal remediation design of a contaminated aquifer. Although this fertilizer management achieves 100% reliability, it is important to note that this strategy is not necessarily the “optimal” policy for 100% reliability. This fact will be further discussed in the section of the mixed-integer stochastic approach (Figure 6.10). The alternative with a 24% reliability level produces a total annual net benefit of 20.8 M€. With 100% reliability (20% fertilizer reduction), the total annual net benefits are reduced to 19.7 M€.

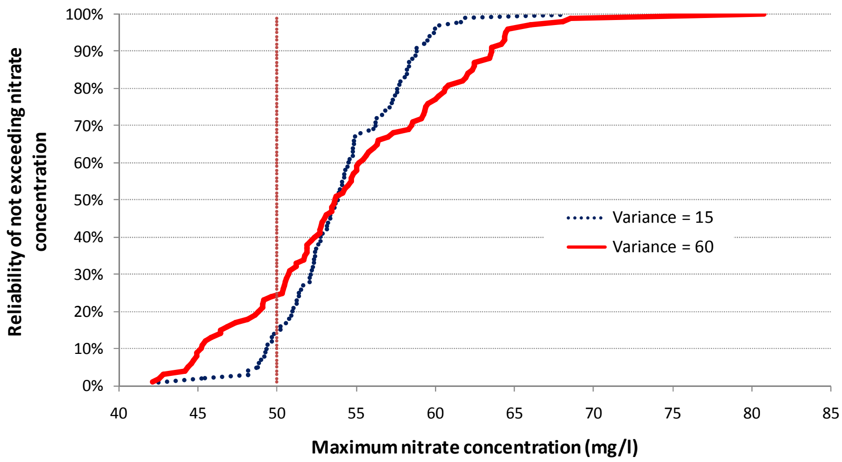


Figure 6.3 Reliability (probability of not exceeding the maximum nitrate concentration) of the optimal fertilizer application for realization 14 with variances of 15 and 60

With this formulation we can analyze the probability of meeting the quality standard for a policy that has been designed without taken into account hydraulic conductivity uncertainty. For this particular example the probability of meeting the quality standard is very low (14 and 24%). It is clear that this reliability levels will highly depend on the realization chosen to find the optimal management (the chosen “true” field).

6.2.4 Monte Carlo optimization

In this formulation, the uncertainty is considered by solving the hydro-economic optimization model for each of the 100 individual realizations and comparing the corresponding results. The results of this approach can be used to characterize the probability distribution of the optimal fertilizer application rates (Figure 6.4). The mean for the case 1 (variance of 15) is 138.3 kg/ha, the standard deviation is 2.9, and the rates range from 131.4 to 148.5 kg/ha. However, we cannot assure that all these strategies would have a high probability of meeting the standard, which limits the applicability to make decisions. In order to estimate the reliability of meeting the objectives of any of the specific strategies that we obtain, we have to simulate the strategy with the complete set of realizations (post-optimality Monte Carlo simulation). For example, if we test the strategy that corresponds to the mean fertilizer application with all the other realizations, we obtain a reliability of meeting the standard of 33%.

For the case 2 (variance of 60), the mean value is 138.9 kg/ha and the standard deviation is 5.3. The reliability of the strategy corresponding to the mean rate is 35%. The results show more dispersivity and a broader range of possible values of the mean fertilizer rates obtained from a single-realization optimization, and therefore, more variability of the economic impact of the strategy, if we have a bigger variance in the K fields.

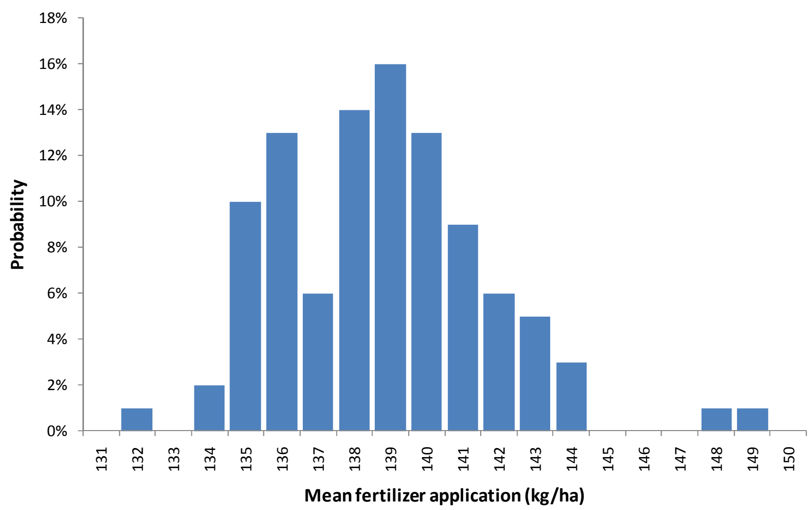


Figure 6.4 Probability distribution of the mean fertilizer application, case 1

6.2.5 Multiple realizations or stacking management model

For this formulation, the hydro-economic management model is solved only once, simultaneously for the complete stack of 100 realizations of the random conductivity field;

therefore, only one optimal fertilizer application is obtained. Chan (1993) investigated the number of realizations to be included in the staking in order to achieve a certain level of reliability, using a Bayesian framework. He obtained the following relationship between stack size (number of realizations, NR) and reliability (R):

$$R = \frac{NR + 1}{NR + 2} \tag{6.7}$$

Feyen and Gorelick (2004) concluded that the previous relationship obtained by Chan (1993) overestimates the reliability for different stack sizes, and presents a formula that provides expected reliability as a function of the number of realizations in the stack and the variance of the log hydraulic conductivity σ^2 as follows:

$$R = \frac{NR - 0.5}{NR + 2\left(\sigma^2 + 1\right)} \tag{6.8}$$

For our case, the application of both equations, (6.7) and (6.8), yields the same reliability for the 100 realizations, 99%. Therefore, the size of the stack is considered big enough to assess reliability levels.

Figure 6.5 shows that, as expected, the water quality standard is not exceeded when simulating the optimal strategy for all the realizations of the stack. The reliability will be therefore 100%, assuming the 100 set of realizations as a representative measure. The total net benefit of the optimal solution with a 100% reliability is higher for case 1 (20.22 M€/year) than for the case with a bigger variance (19.89 M€/year), since in the latter the fertilizer application has to be lower in order to meet the standards. The use of this approach does not allow for prespecification of the desired system reliability. Since the reliability of the system management is not explicitly considered in the optimal solution, the method can lead to conservative (and more expensive) solutions.

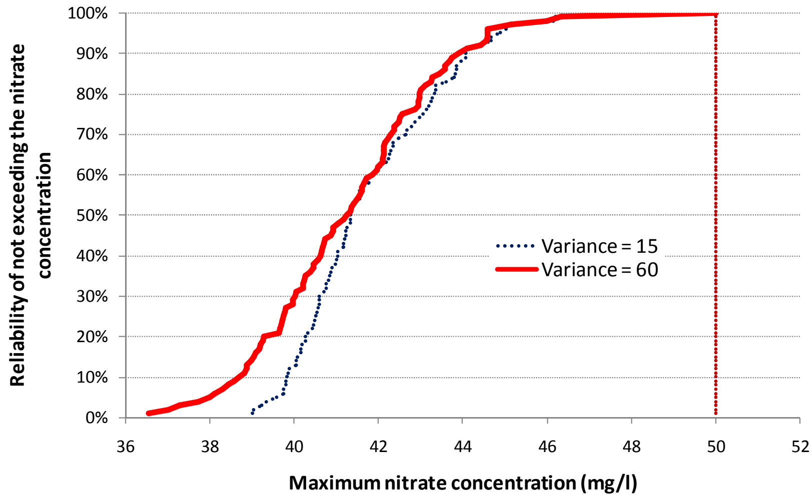


Figure 6.5 Maximum nitrate concentration vs. reliability of not exceeding the nitrate concentration (post Monte Carlo simulation)

To analyze the influence of the stack size in the reliability of the resulting strategies (Figure 6.6), we found the optimal solutions of the multiple realization models for stack sizes of 2, 5, 10, and 30 realizations. Post-optimization Monte Carlo reliability analyses are carried out by simulating each optimal solution against the set of a hundred different hydraulic conductivity realizations. Figure 6.7 shows the mean reliability for all the possible stacks of equal size. As expected, the reliability of the optimal solution increases with the size of the stack considered to find the fertilizer rate. The mean values of reliability vs. stack size are in agreement with the findings of Wagner and Gorelick (1989), Chan (1993), and Ko and Lee (2009) for the optimal remediation design to control groundwater pollution, and Feyen and Gorelick (2004) for controlling groundwater outflow in wetlands. We can obtain a high reliability with a stack of a reduced number of realizations.

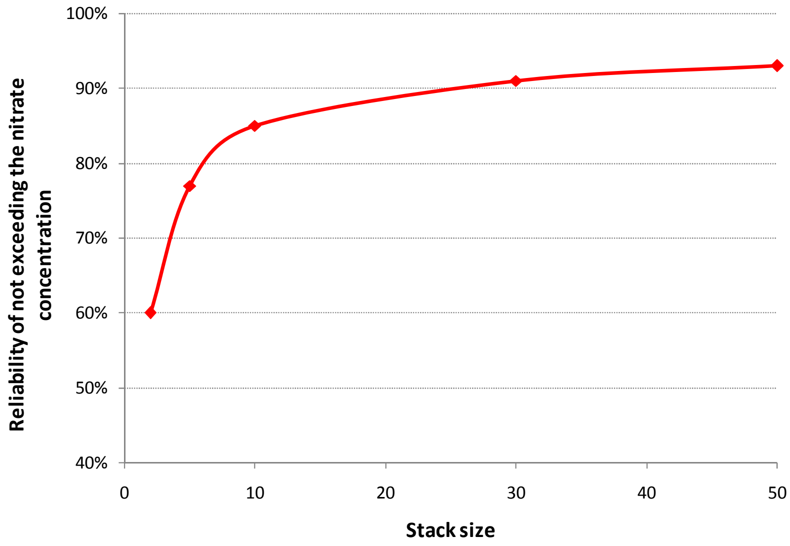


Figure 6.6 Mean reliability (post Monte Carlo simulation) vs. stack size

6.2.6 Mixed-integer stochastic model with predefined reliability

In this formulation, the stochastic nature of the conductivity field was considered in the decision-making process by integrating the complete set of Monte Carlo realizations through the response matrix of the optimization management model. The method allows for prespecification of the desired system reliability. It also guarantees the optimal solution for this reliability value, since it simultaneously uses all the generated realizations. The desired reliability of the system is predefined by fixing the number of constraints that may be violated. Different reliability levels were tested. The range of the maximum concentration values that are reached decreases with increasing reliability, and a steeper slope of the probability curve is observed (Figure 6.7). However, the worst-case (upper value) of the maximum nitrate concentrations increases with decreasing reliability (Figure 6.8). The bigger the variance, the greater the range and the worst-case (maximum concentration values). We also infer from Figure 6.8 that the bigger the variance of the uncertain parameter, the greater the maximum concentration that can be reached for the same level of reliability of meeting the water quality standard. Again, this implies that, with a high variance, a risk-averse decision-maker would prefer a strategy with a higher reliability to avoid the risk of a high nitrate concentration exceeding by far the standard (which will implies higher economic impacts in terms of environmental and resource cost).

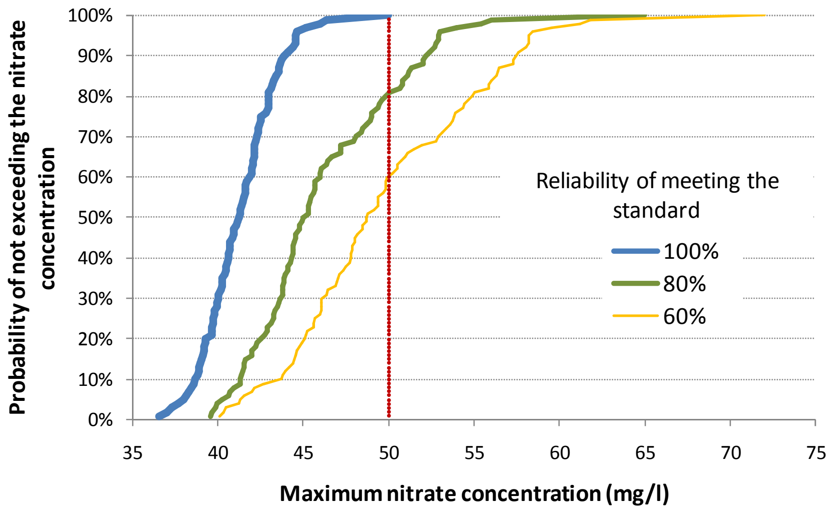


Figure 6.7 Probability of not exceeding the nitrate concentration for different reliability levels (case 2).

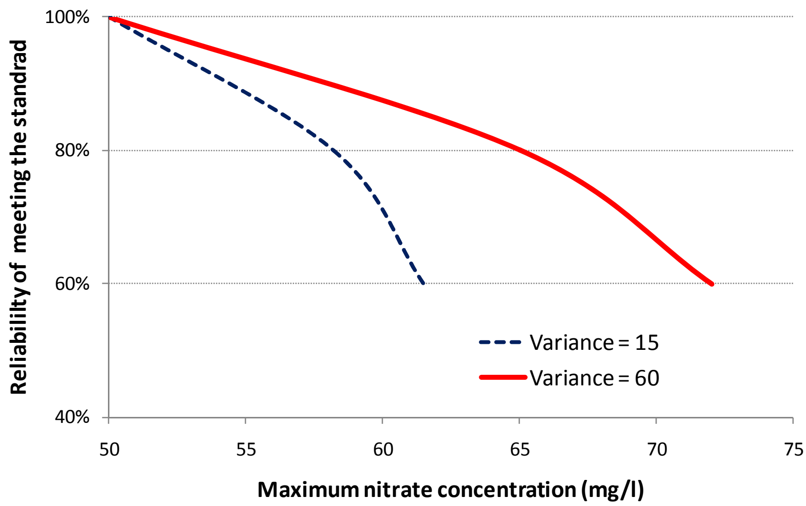


Figure 6.8 Reliability vs upper value of maximum nitrate concentrations

Figure 6.9 shows that the objective function (the total net benefit) increases nonlinearly with decreasing reliability. This implies that a larger amount of net benefit has to be sacrificed if we consider more risk-averse management.

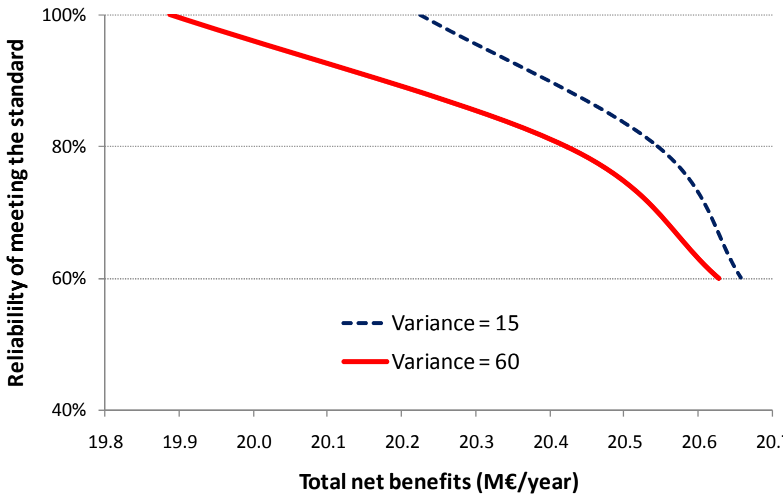


Figure 6.9 Trade-off between reliability and benefits.

For the same reliability level, the total net benefit is greater when the variance is lower. A high variance also implies that some critical realizations further limit the fertilizer application rate for that reliability level. As the reliability level gets lower, the total net benefit for both K variance fields gets closer, since the fertilizer rate moves toward the optimal application that yields the maximum benefits.

Figure 6.10 shows the performance of the different approaches for dealing with the parameter uncertainty. All the other solutions are more costly or less reliable than the solutions generated by the mixed-integer stochastic model with predefined reliabilities, and are therefore all inferior solutions; these results are also in agreement with Morgan et al. (1993).

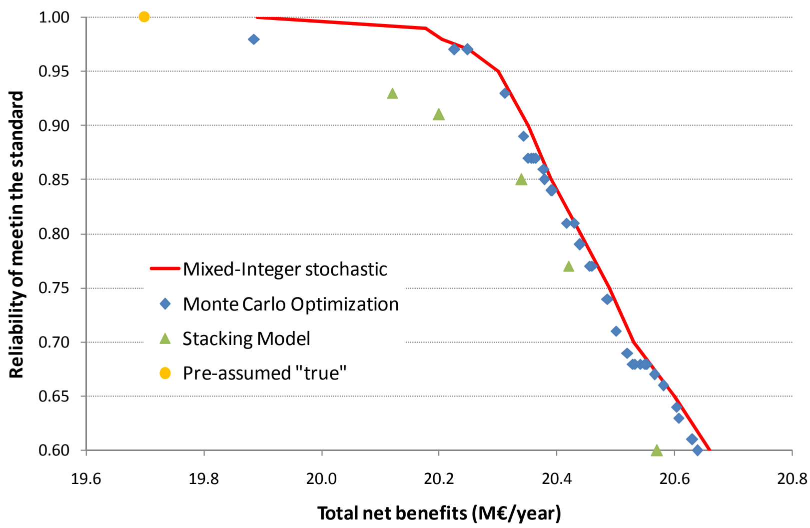


Figure 6.10 Comparison between the solutions of the different formulations

Another important feature of this framework is that the optimal spatial fertilizer application is also obtained. For each realization the influence of the different sources upon the concentration at the control sites might be different, and the corresponding benefits from crop production differ. Table 6.1 shows the percentage of fertilizer reduction from the loading that produces the maximum crop yield that is required to meet the ambient quality for different levels of reliability. These results can be relevant for the design of optimal land use policies to control groundwater nitrate pollution. From the table we can see that no fertilizer reduction is need in certain areas, while in the other areas the reduction has to be greater in order to achieve a higher reliability of meeting the standards. The pattern of the spatial fertilizer reduction is maintained for the different reliability levels, showing the robustness of the solution.

Table 6.1 Percentage of spatial fertilizer reduction for different levels of reliability

Crop Area	Reliability		
	100%	**80%**	**60%**
s1	3.29%	2.58%	2.12%
s2	0.00%	0.00%	0.00%
s3	43.07%	29.22%	22.17%
s4	0.00%	0.00%	0.00%
s5	17.99%	14.00%	11.48%
s6	2.75%	2.15%	1.76%
s7	0.00%	0.00%	0.00%

6.3 Discussion

In this chapter four different formulations (Monte Carlo simulation with preassumed parameter field, Monte Carlo optimization, stacking approach, and mixed-integer stochastic optimization with predefined reliability level) have been applied in order to analyze the influence of the uncertainty of the spatial variability of the hydraulic conductivity upon the optimal management of groundwater nitrate pollution from agricultural sources. All the approaches use a Monte Carlo-type analysis involving a series of realizations of the uncertain parameter, in order to assess reliability and uncertainty of different fertilizer application strategies. The framework has been applied to a controlled 2D synthetic aquifer system, offering insights into the impacts of uncertainty in the optimal management strategies.

Given the uncertainty in the pollutant concentration predictions due to uncertain in the spatial variability of the hydraulic conductivity, the solution of the optimization of a single realization does not guarantee a high reliability in meeting the groundwater quality standards. Using Monte Carlo simulation, we obtained that the strategy derived from a single realization assumed as a “true” parameter field yields a very low reliability in meeting the standard. Although we can reduce the constraining quality standard in order to achieve a higher reliability, it has been proved that this solution does not necessarily yield the maximum for the objective function (total net benefits). A stochastic analysis that considers uncertainty in the performance of the system allows providing more reliable management strategies than deterministic models.

In order to increase the reliability, we can simultaneously optimize for a sampling or stack of hydraulic conductivity realizations (stacking approach). It has been shown that the reliability of the optimal solution increases with the stack size. However, this approach does not allow for pre-specification of the desired system reliability. Since the reliability is not explicitly considered in the optimal solution, the method can lead to too conservative solutions.

However, in decision-making processes, reliability and risk-aversion play a decisive role. By using a mixed-integer stochastic formulation, an a priori reliability level of the strategy can be explicitly fixed. As the mixed-integer stochastic model includes the complete set of realizations, it guarantees the best optimal strategy (maximum total net benefit) for that level of reliability, as shown by the results. This approach also allows deriving the trade-off curve between the reliability level and the net benefits.

In a risk-averse decision-making, not only the reliability of meeting the standards counts, but also the probability distribution of the maximum pollutant concentrations. A risk-averse decision-making is specially justified when dealing with well-capture zones for drinking water supply (health risk) or sensitive areas of groundwater dependent ecosystems. A sensitivity analysis was conducted to assess the influence of the variance of the hydraulic conductivity fields on the optimal strategies. The results have shown that the bigger the variance, the greater the range of maximum nitrate concentrations and the worst-case (or maximum value) that could be reached for the same level of reliability of meeting the standard.

In the reliability vs. net benefit trade-off, for the same reliability level, the total net benefit is greater when the variance is lower. Note that by assuming uncertainty in the random function (e.g., Llopis-Albert and Capilla, 2009) or by considering higher variances of the K, a greater influence in the results than in the analyzed cases should be expected.

The probability distribution of the fertilizer application rate can be assessed by Monte Carlo optimization, solving the optimization problem for each of the individual realizations. The results obtained for the illustrative example shows that the strategy corresponding to the mean rate yields a low reliability in meeting the quality standard. The K variance increases the standard deviation of the mean rates probability distribution.

7 Conclusions, limitations and future research

7.1 Summary and conclusions

In recent decades, nitrate concentrations in groundwater have increased due mainly to the intensive use of fertilizers in agriculture in order to boost the crop yields. In Europe, the EU water legislation establishes a limit of nitrate concentration in groundwater bodies of 50 mg/l (the quality limit for drinking water supply), and requires that groundwater bodies reach a good quantitative and chemical status by year 2015. In addition, any significant upward trend in the concentration of any pollutant should be identified and reversed (Directive 2006/ 118/EC, Groundwater Directive). To control groundwater diffuse pollution, it is necessary to analyze and implement management decisions.

This thesis 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 rates that maximize 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. They are used to translate the 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 first applied to a synthetic case study 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.

The method has been also applied to a real case study, the Salobral-Los Llanos aquifer (within the Mancha Oriental groundwater body). The results show the fertilizer reduction represent an average decrease in the net benefits of about 12 M€/year with regard to the expected benefit under the baseline scenario. Additionally, the farmer's response to an increase in the fertilizer price was simulated. An extremely high price would be required to reduce the fertilizer use so that nitrate concentrations in groundwater stay below the 50 mg/l. These results show that it is more cost-efficient to apply standards to fertilizer use than taxes. However, the instrument of fertilizer standards is more difficult to implement and control. The use of fertilizer taxes constitutes a promising policy instruments that need to be further explored.

Given the uncertainty in the pollutant concentration predictions, it has been shown that the solution of the optimization for a single realization of the groundwater hydraulic parameters does not guarantee a high reliability in meeting the groundwater quality standards. A stochastic modeling framework was developed in order to analyze the influence of the uncertainty on the spatial variability of the hydraulic conductivity field. Four different formulations, based on a Monte Carlo-type analysis involving a series of realizations of the uncertain parameter, were applied to a synthetic case study in order to assess reliability and uncertainty of different fertilizer application strategies. In order to increase the reliability of the solution, several realizations can be optimized at the same time. It has been shown that the reliability level is affected by the stack size. By using a mix-integer stochastic formulation, an apriori reliability level of the strategy can be explicitly fixed. As the mixed-integer stochastic model includes the complete set of realizations, it guarantees the best optimal strategy (maximum aggregated net benefit) for that level of reliability. This approach also allows deriving the trade-off curve between the reliability level and the net benefits.

The method presented can contribute to implementing the EU Water Framework Directive by providing insights for the definition of cost-efficient policies or programme of measures to control diffuse groundwater pollution. The modeling framework allows estimation of the opportunity cost (as forgone benefits) 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.

7.2 Limitations and recommendations for future research

This thesis has demonstrated that the methodology developed provides a valuable framework to analyze different policy options to reduce nitrate concentrations in groundwater. However, some improvements can be made. Listed below are some recommendations for future research.

- Incorporate the water use into the decision variables. Often when farmers reduce fertilizer application they also reduce the use of other inputs (pesticides, irrigation) in order to maximize their net income. The main problem to be addressed in this sense is that, when the amount of irrigation water applied varies, the recharge to the aquifer also changes, creating non-linearities and making the superposition method not suitable (thus, the response matrix approach will not be applicable).
- Farmers may decide to stop producing one crop or switch to another one, in response to change in prices. In order to be able to simulate this, the optimization scheme should allow modifying crop patterns and crop location, including crops into the decision variables.
- 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 modeling the economics of abating the pollution from these other sources.
- The uncertainty in pollutant transport simulation can be reduced by improving the site characterization and providing more realistic and reliable management schemes. For that purpose, a promising extension of the present work is the integration of a stochastic inverse model in the described framework, in which the stochastic simulations are constrained to data such as hydraulic conductivity,

piezometer head, solute concentrations, travel times or secondary data obtained from expert judgment and geophysical surveys.

- Besides groundwater hydraulic conductivity there are many other sources of uncertainty, ranging from partial knowledge about the aquifer properties and boundary conditions, land use practices, on-ground nitrogen loading, nitrogen soil dynamics, soil characteristics, depth to water table, to the diverse economic, regulatory and political factors. Further research is required to extend the analysis to other sources of uncertainty.
- Only the policies of fertilizer standards and fertilizer taxes are analyzed. A broad range of policies for controlling nitrates has been discussed in the literature (including standards or different economic instruments applied to inputs, emissions or ambient concentrations) (e.g. Shortle and Griffin, 2001). A further extension of this work is to incorporate these different policies into the hydro-economic formulation in order to compare their effectiveness in controlling nitrate pollution as second-best solutions.
- In this analysis, the cost of the policies for controlling nitrate pollution is simplified as the direct costs to the users, in terms of net income losses. Transaction costs associated with introducing and maintaining a policy instrument are not considered, although they might be significant in certain cases.

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Appendix A. Crop yield and nitrate leaching functions. El Salobral-Los Llanos Case Study

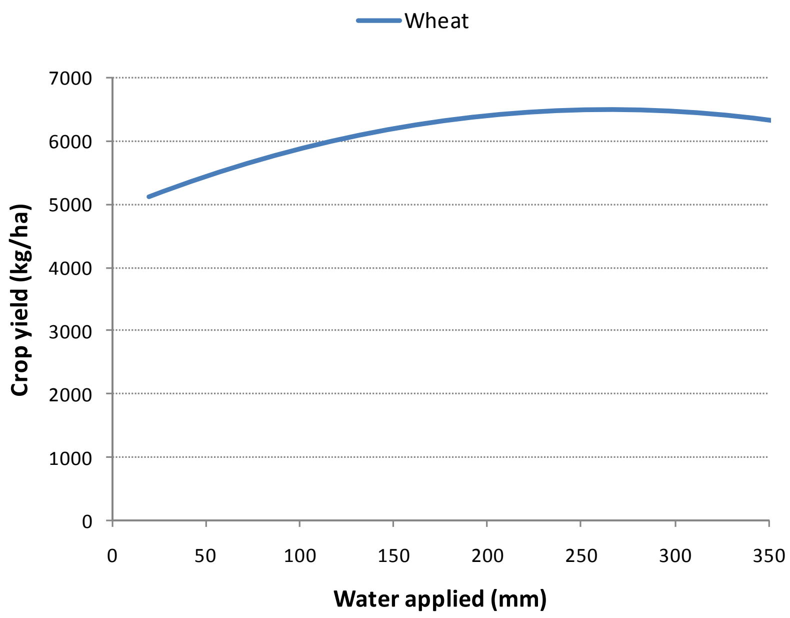

Figure A.1. Wheat yield vs. water application

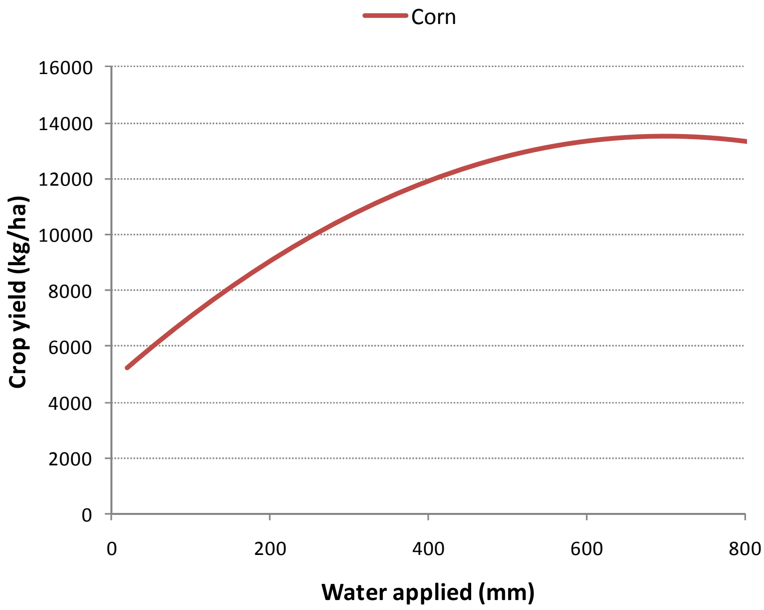

Figure A.2. Corn yield vs. water application

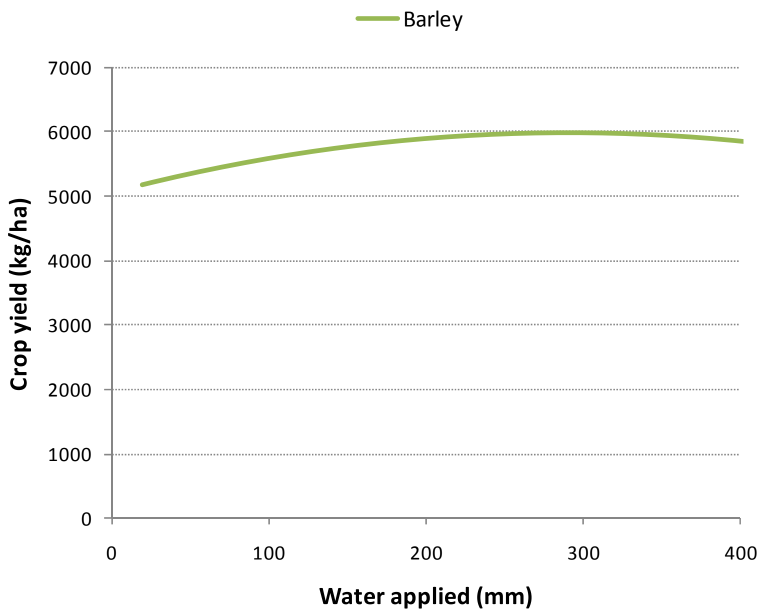

Figure A.3. Barley yield vs. water application

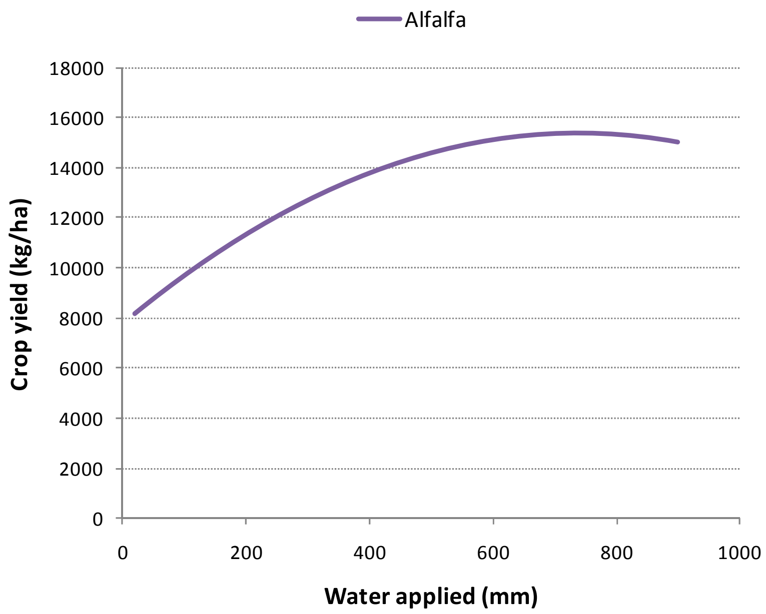

Figure A.4. Alfalfa yield vs. water application

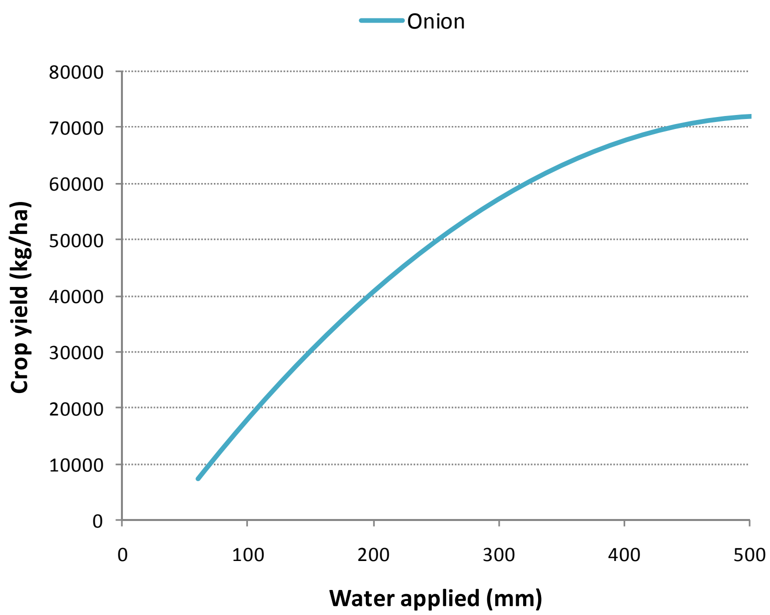

Figure A.5. Onion yield vs. water application

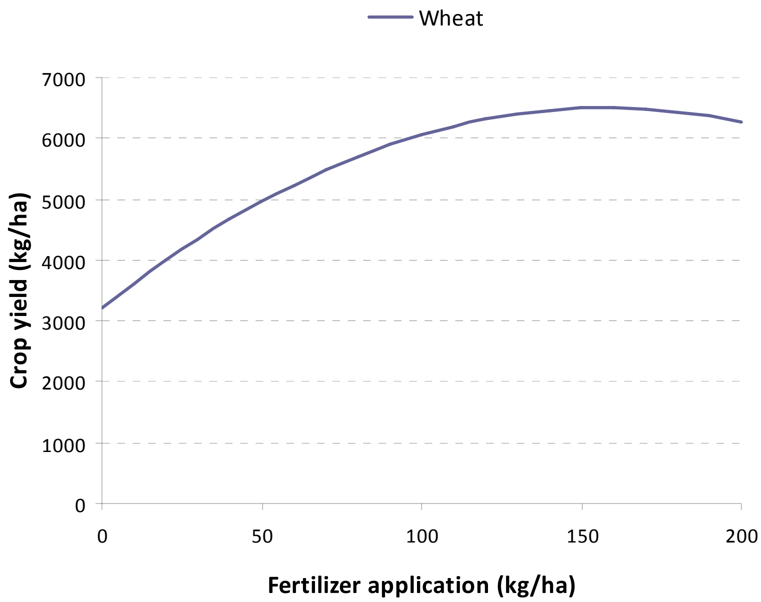

Figure A.6. Wheat yield vs. fertilizer application

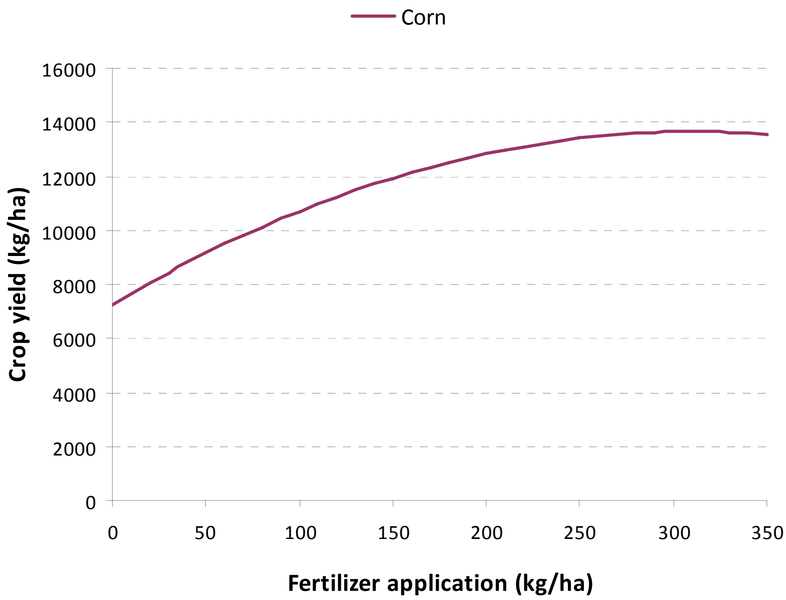

Figure A.7. Corn yield vs. fertilizer application

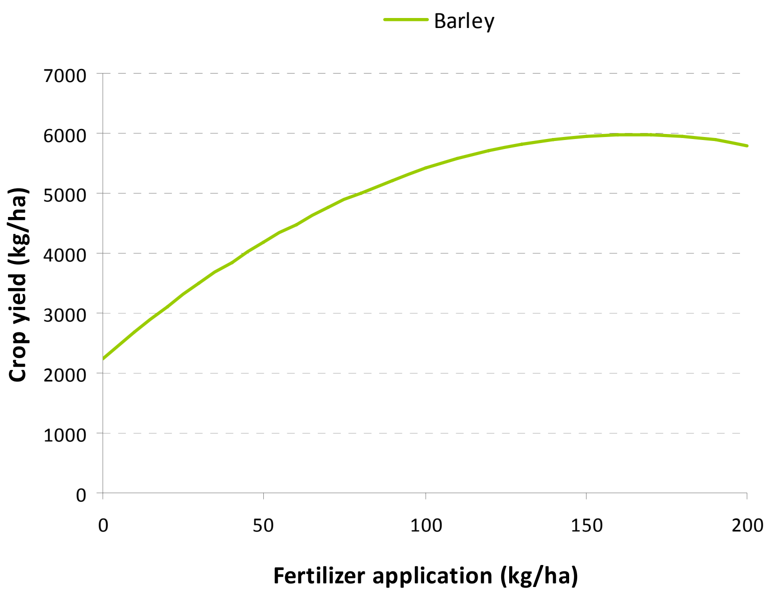

Figure A.8. Barley yield vs. fertilizer application

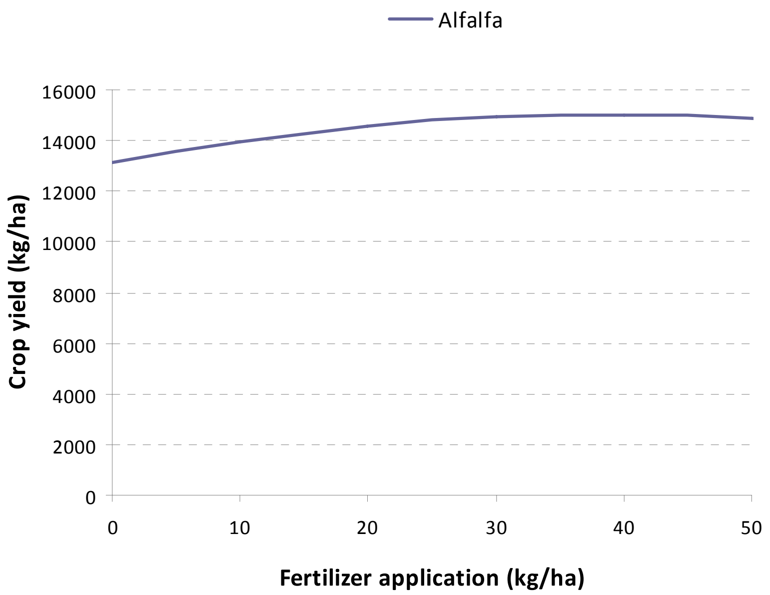

Figure A.9. Alfalfa yield vs. fertilizer application

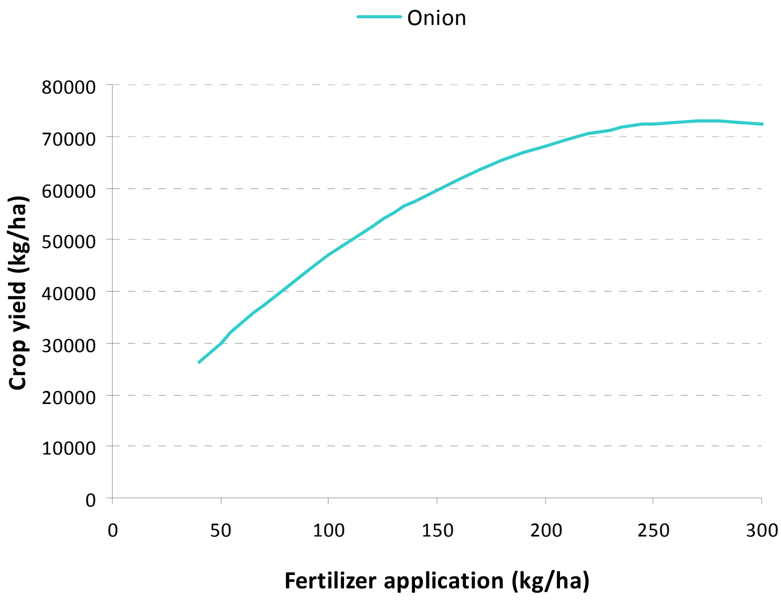

Figure A.10. Onion yield vs. fertilizer application

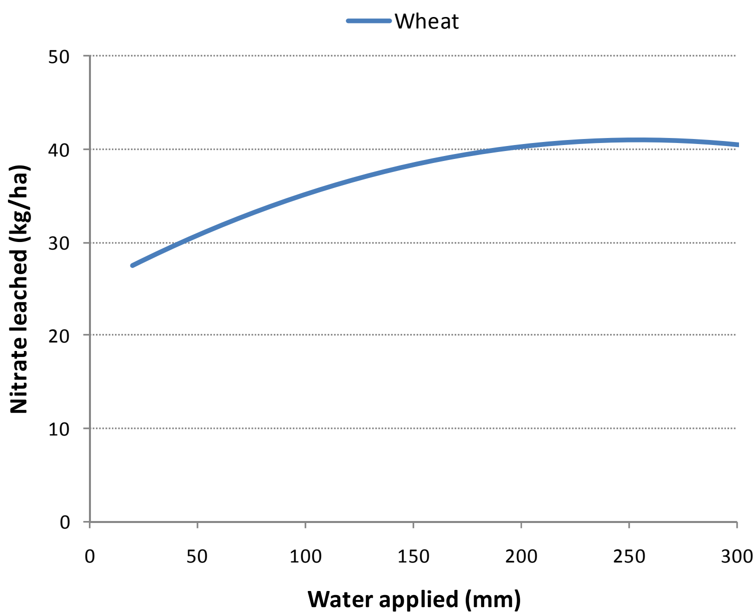

Figure A.11. Nitrate leaching vs. water application on Wheat

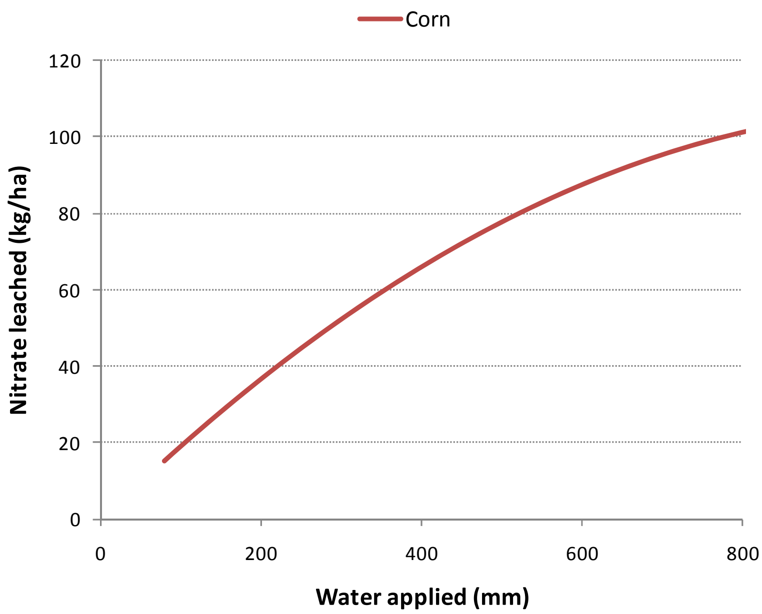

Figure A.12. Nitrate leaching vs. water application on Corn

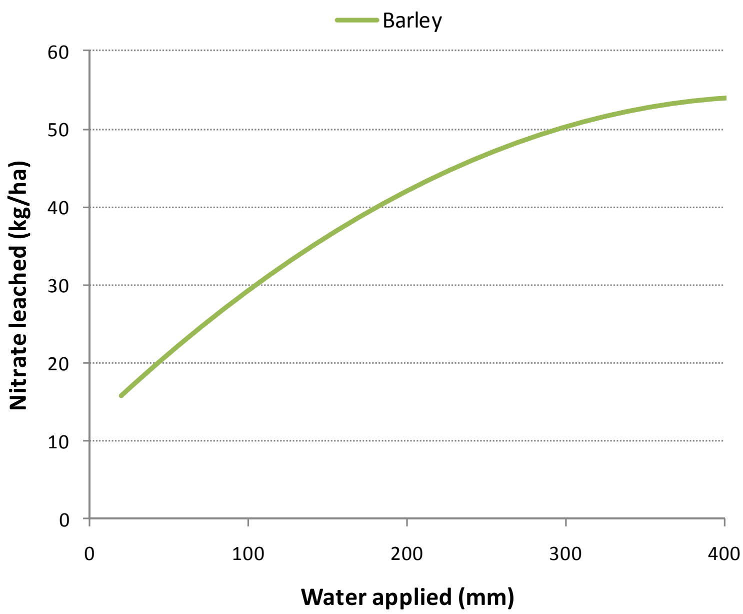

Figure A.13. Nitrate leaching vs. water application on Barley

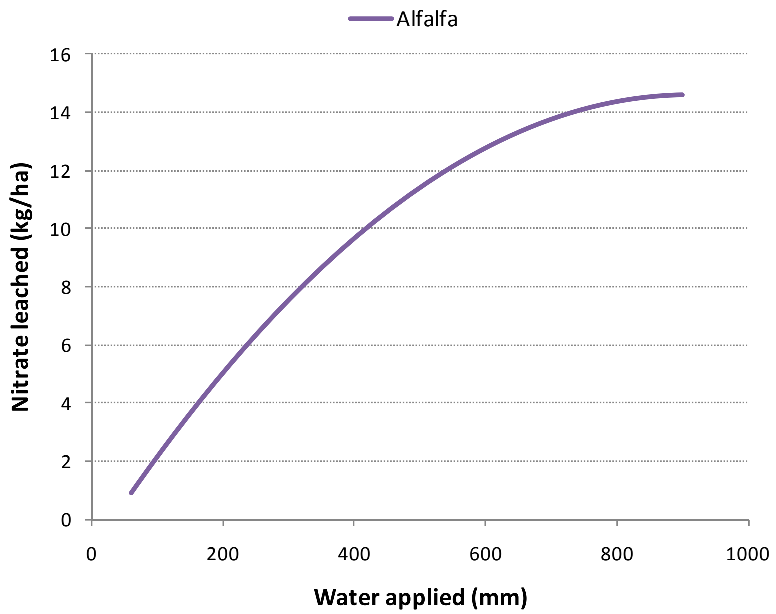

Figure A.14. Nitrate leaching vs. water application on Alfalfa

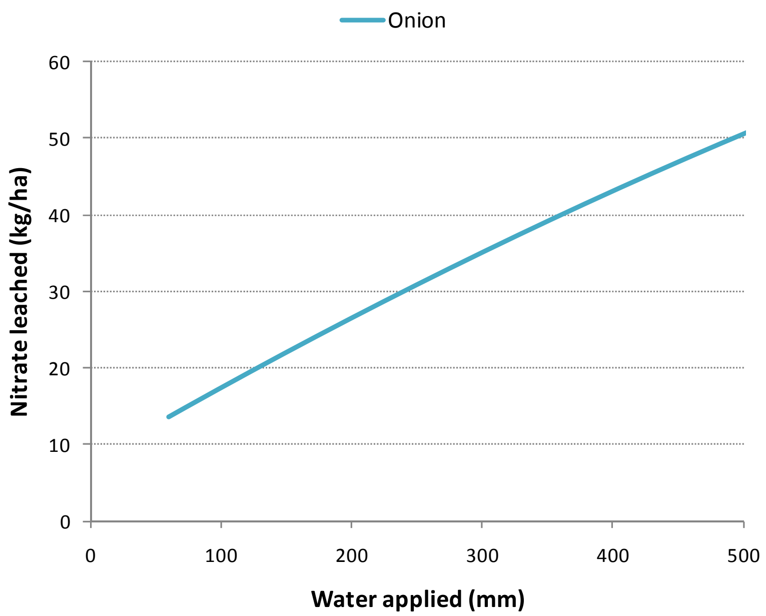

Figure A.15. Nitrate leaching vs. water application on Onion

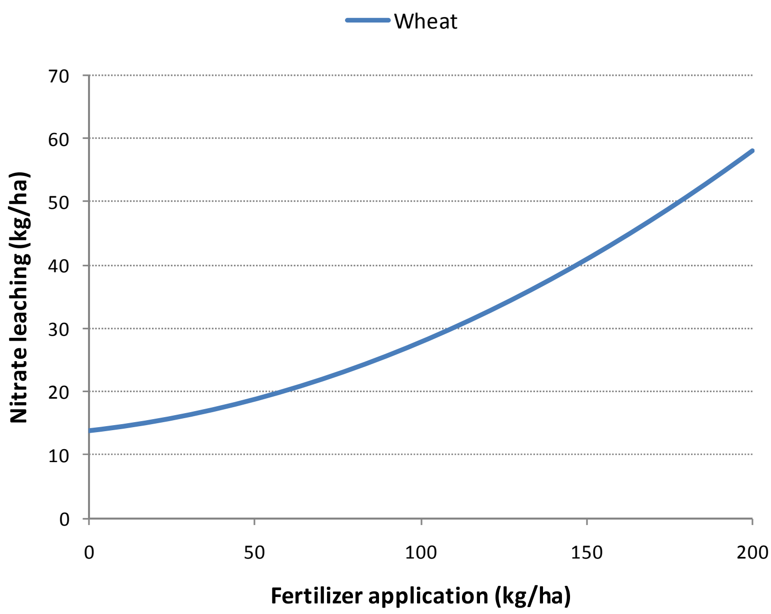

Figure A.16. Nitrate leaching vs. fertilizer application on Wheat

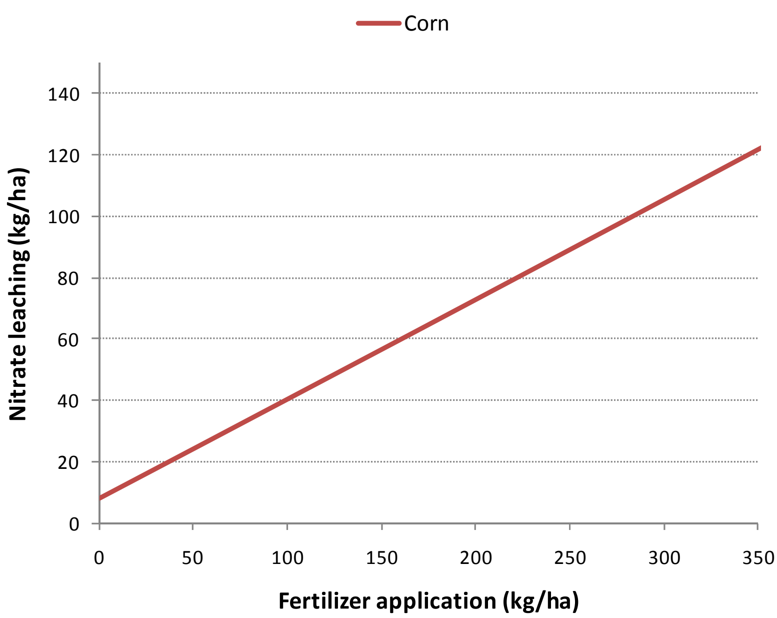

Figure A.17. Nitrate leaching vs. fertilizer application on Corn

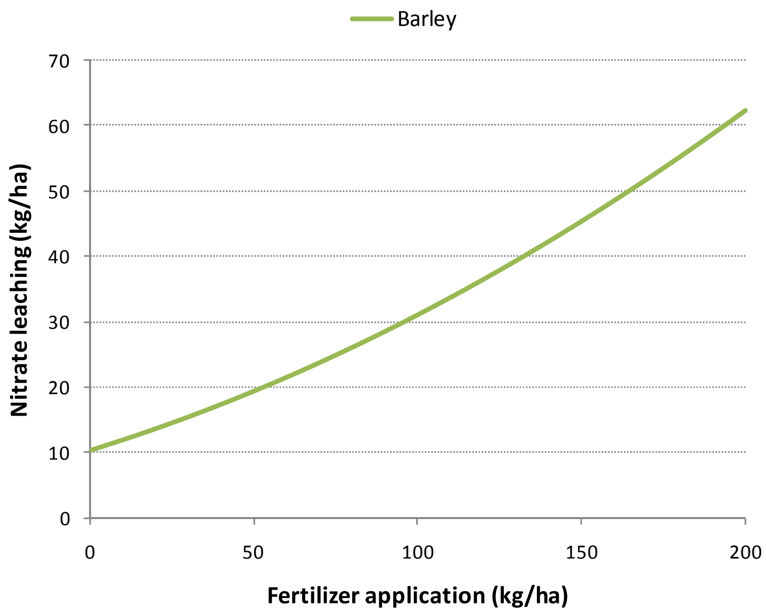

Figure A.18. Nitrate leaching vs. fertilizer application on Barley

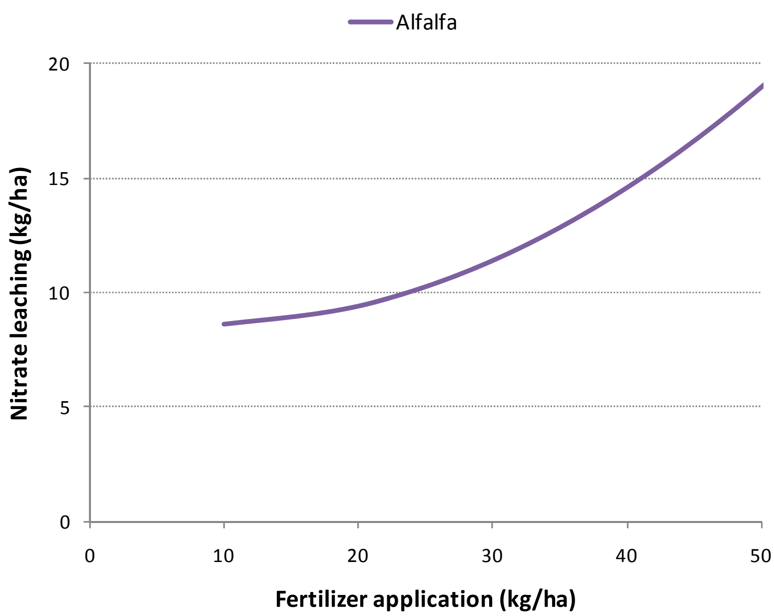

Figure A.19. Nitrate leaching vs. fertilizer application on Alfalfa

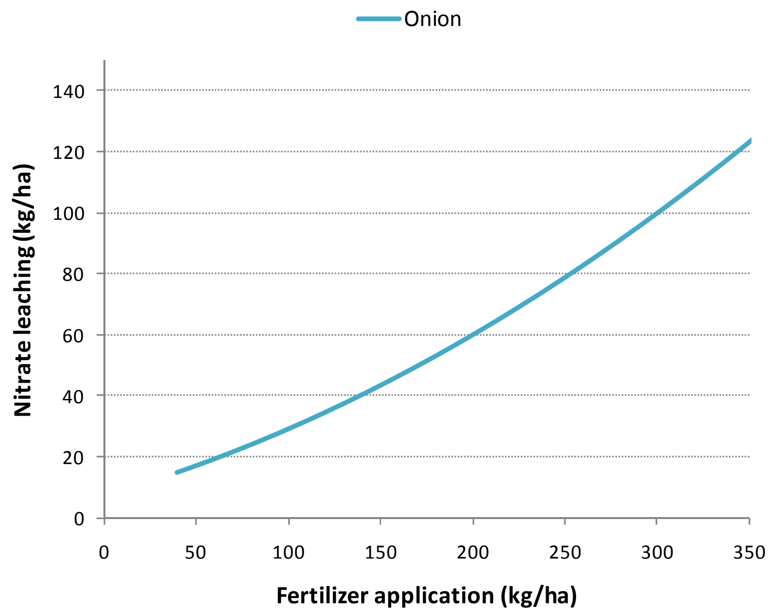

Figure A.20. Nitrate leaching vs. fertilizer application on Onion

Appendix B. Groundwater flow model calibration. El Salobral-Los Llanos case study

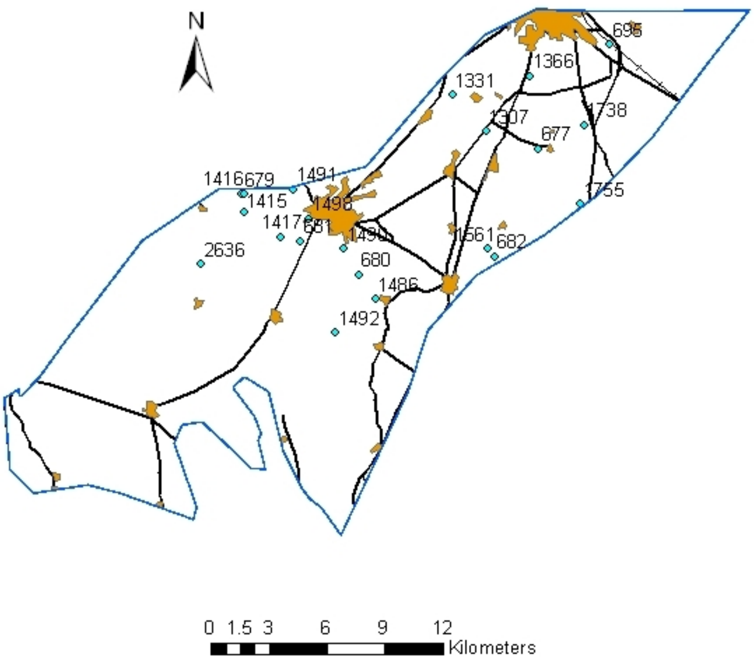

Figure B.1. Location of the observation wells

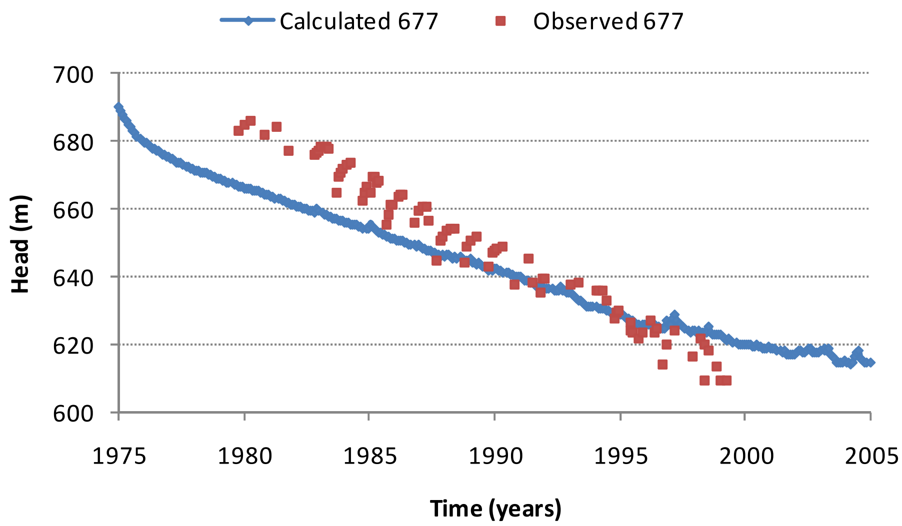

Figure B.2. Calculated vs. measured heads in wells 677

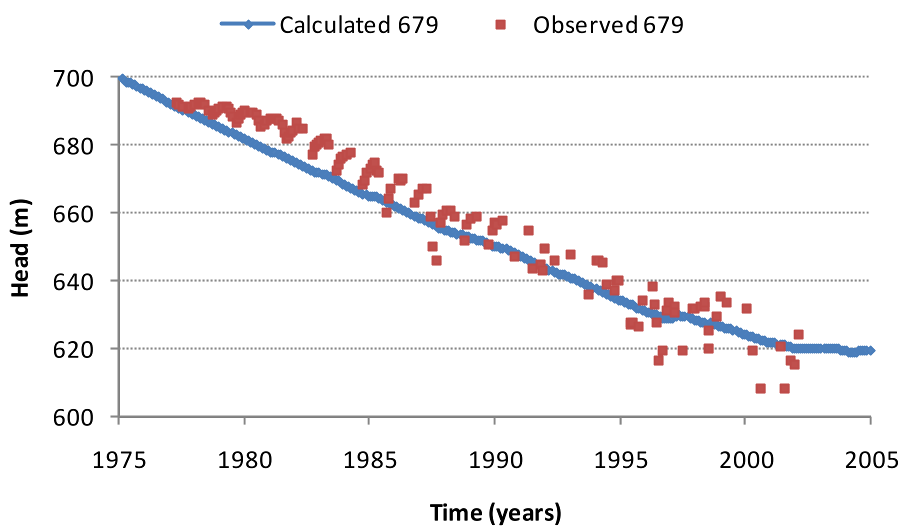

Figure B.3. Calculated vs. measured heads in wells 679

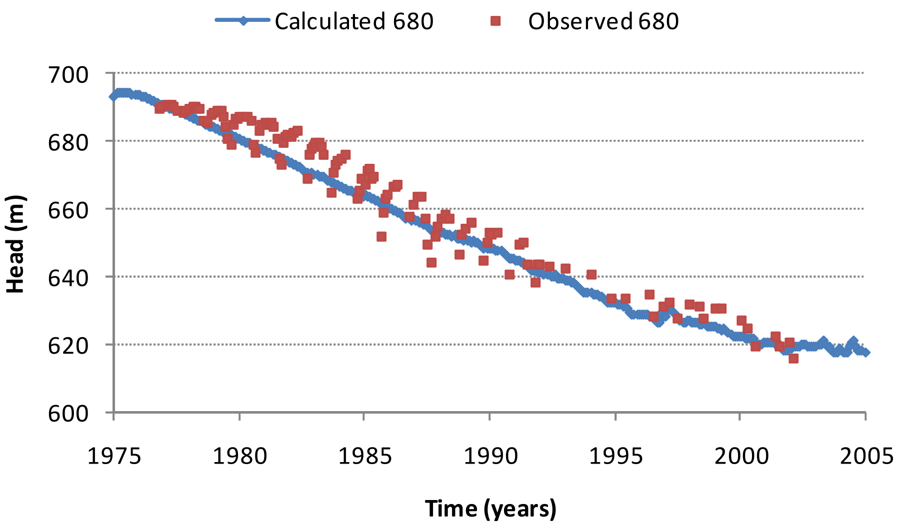

Figure B.4. Calculated vs. measured heads in wells 680

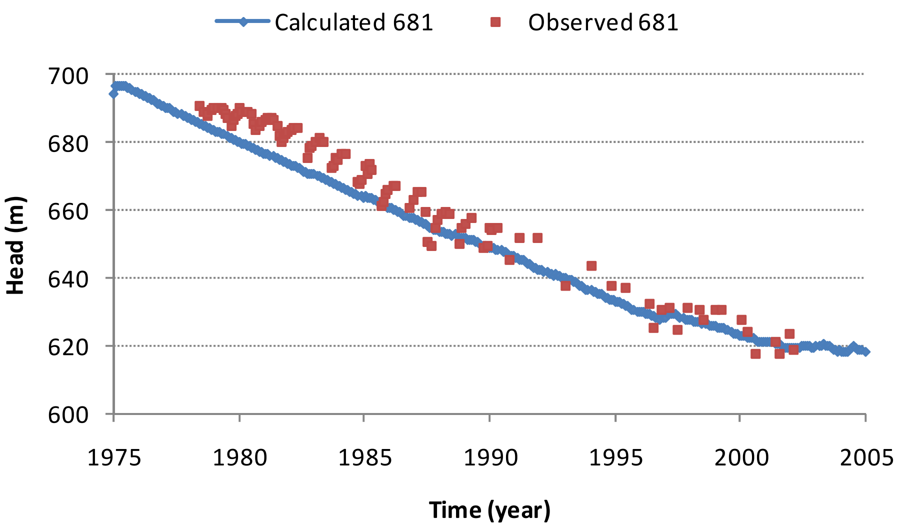

Figure B.5. Calculated vs. measured heads in wells 681

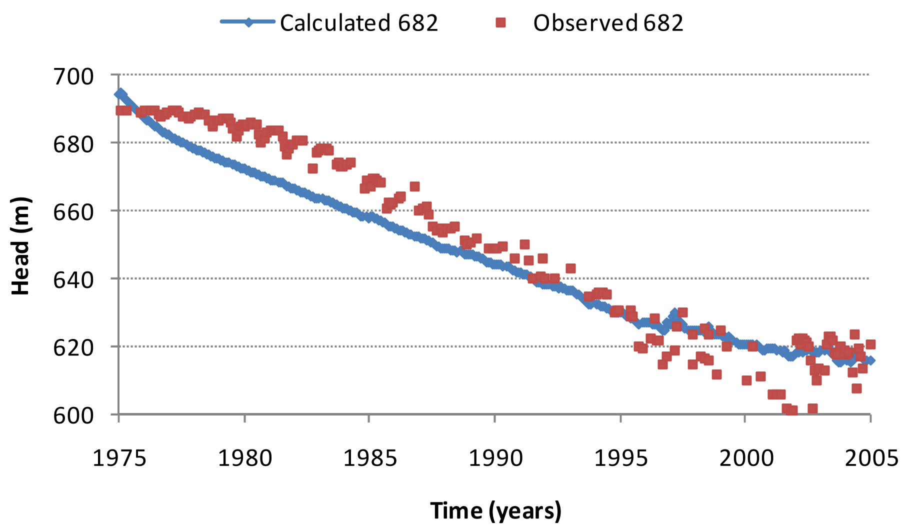

Figure B.6. Calculated vs. measured heads in wells 682

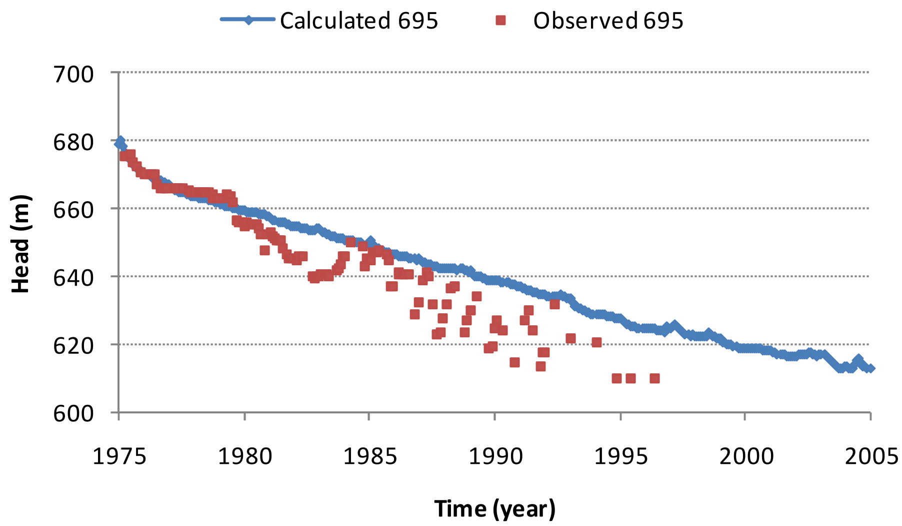

Figure B.7. Calculated vs. measured heads in wells 695

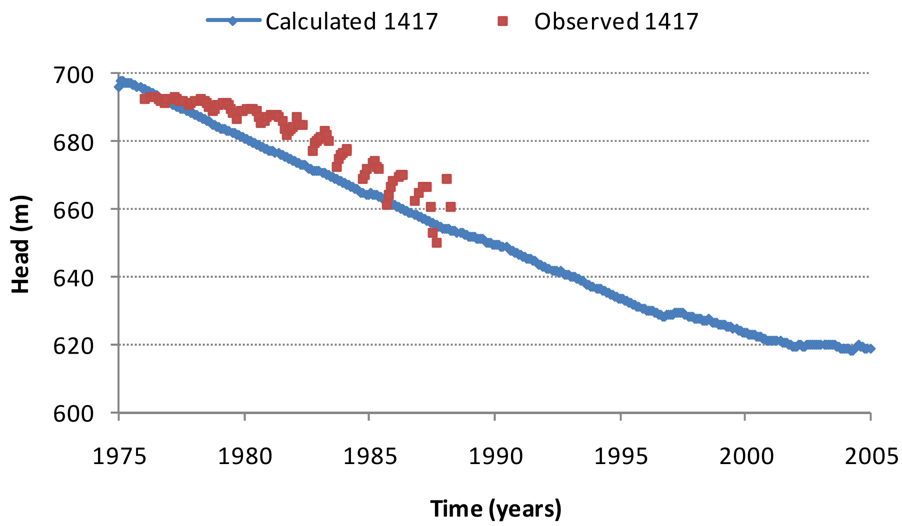

Figure B.8. Calculated vs. measured heads in wells 1417

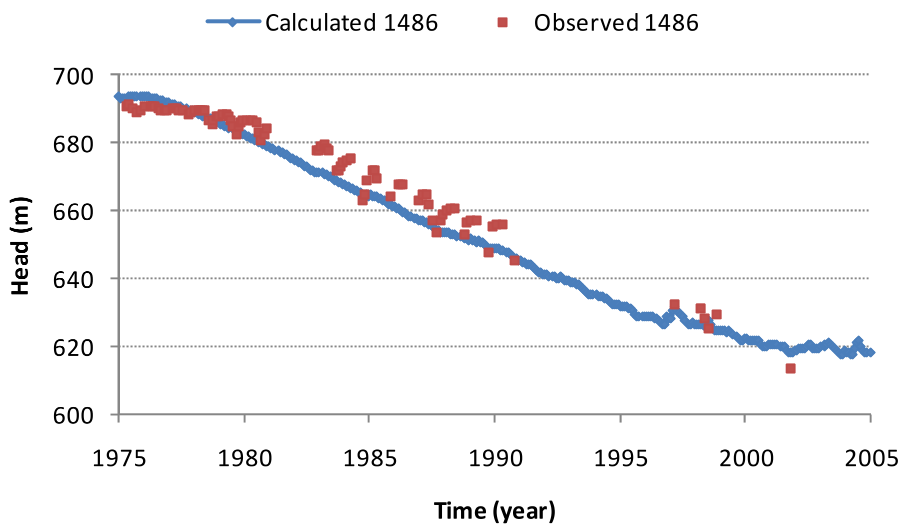

Figure B.9. Calculated vs. measured heads in wells 1486

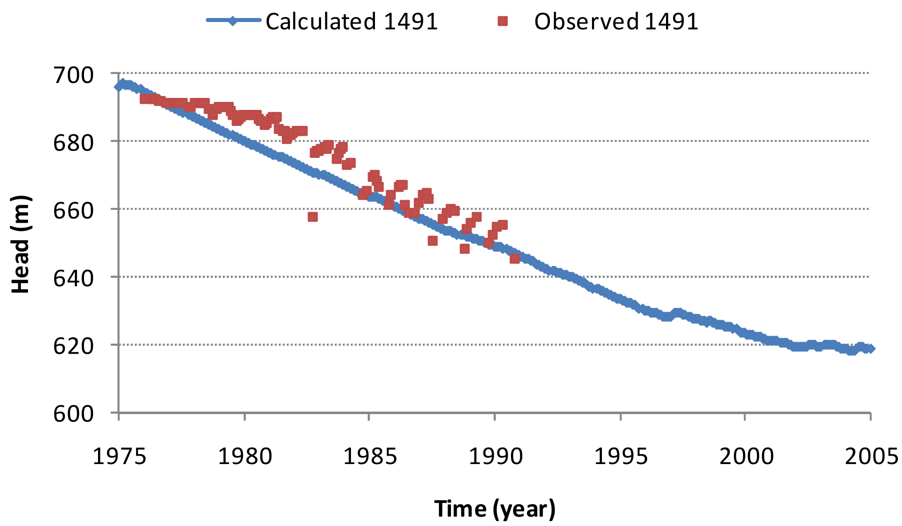

Figure B.10. Calculated vs. measured heads in wells 1491

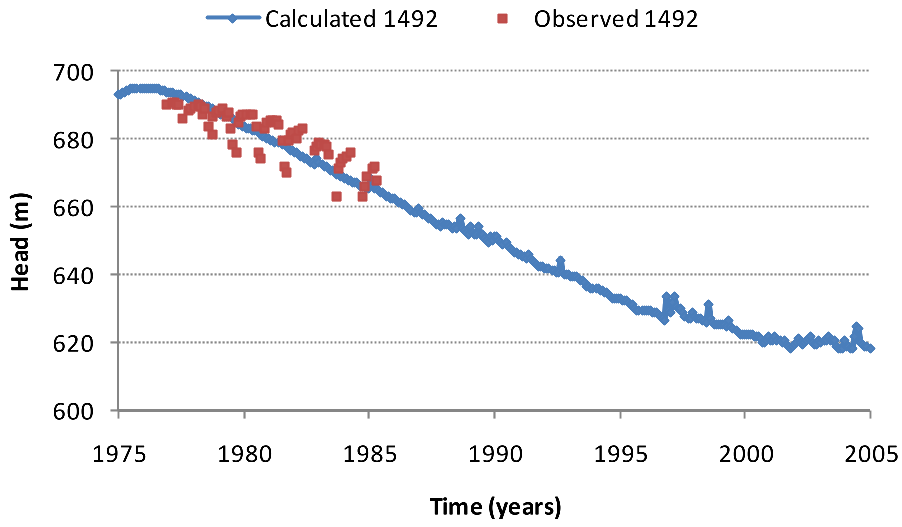

Figure B.11. Calculated vs. measured heads in wells 1492

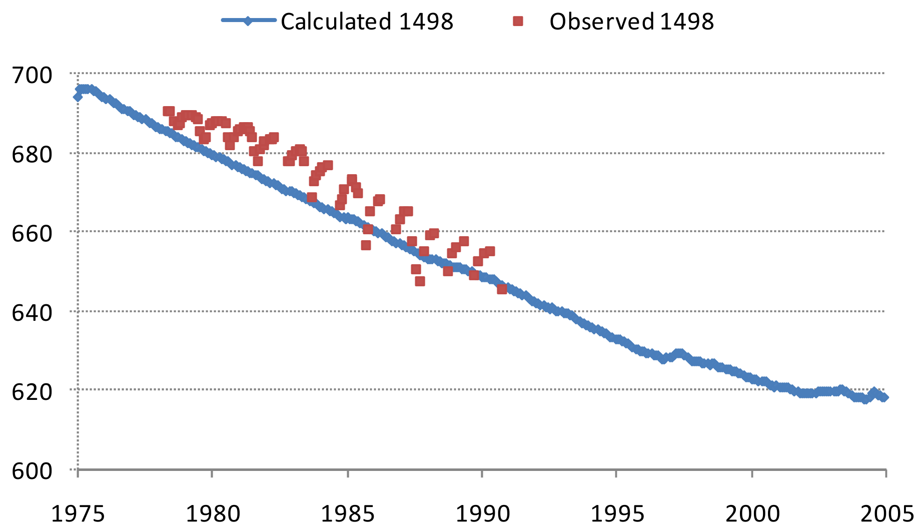

Figure B.12. Calculated vs. measured heads in wells 1498

Appendix C. Unitary nitrate concentration curves. El Salobral-Los Llanos case study.

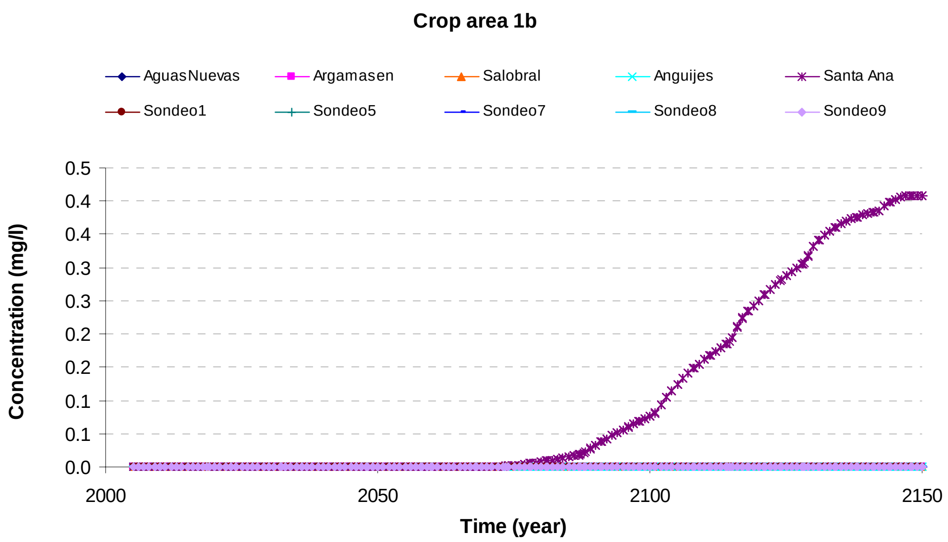

Figure C.1 Unitary concentration-time curves for crop area 1b

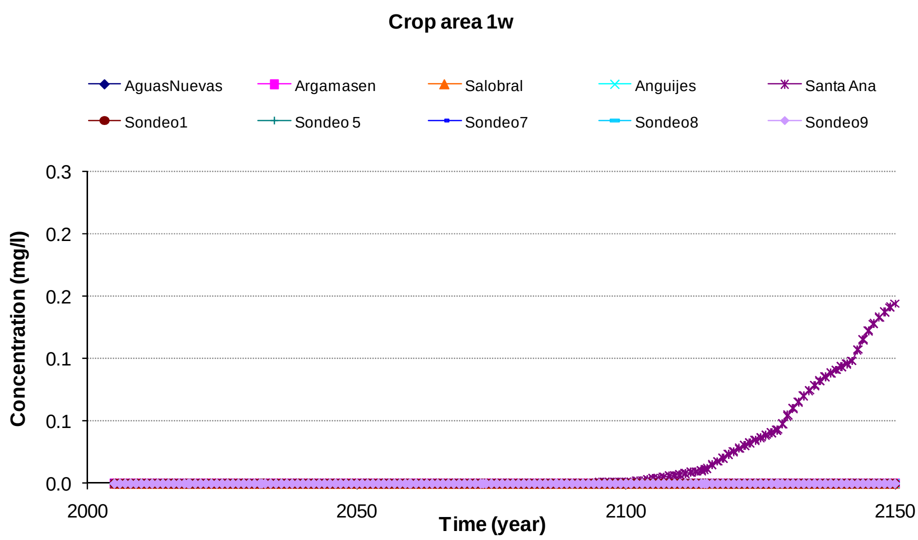

Figure C.2 Unitary concentration-time curves for crop area 1w

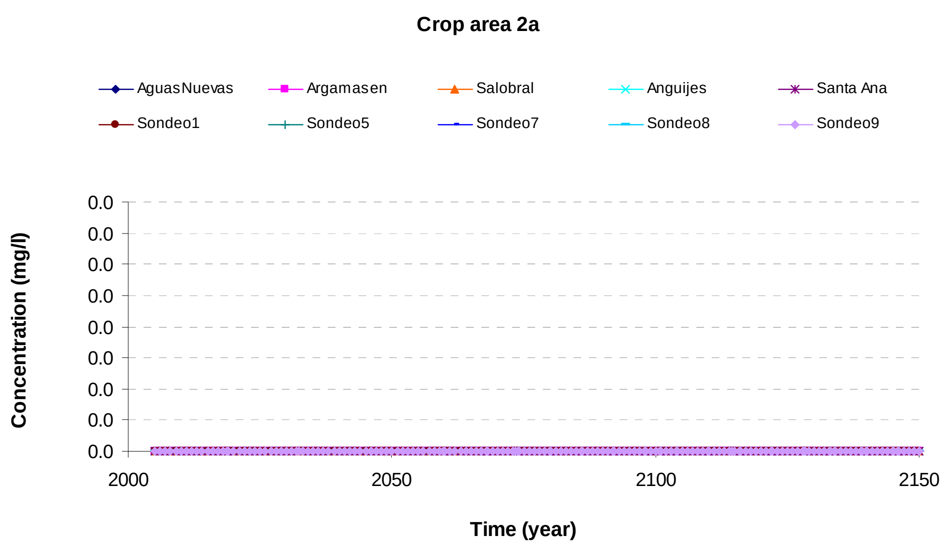

Figure C.3 Unitary concentration-time curves for crop area 2a

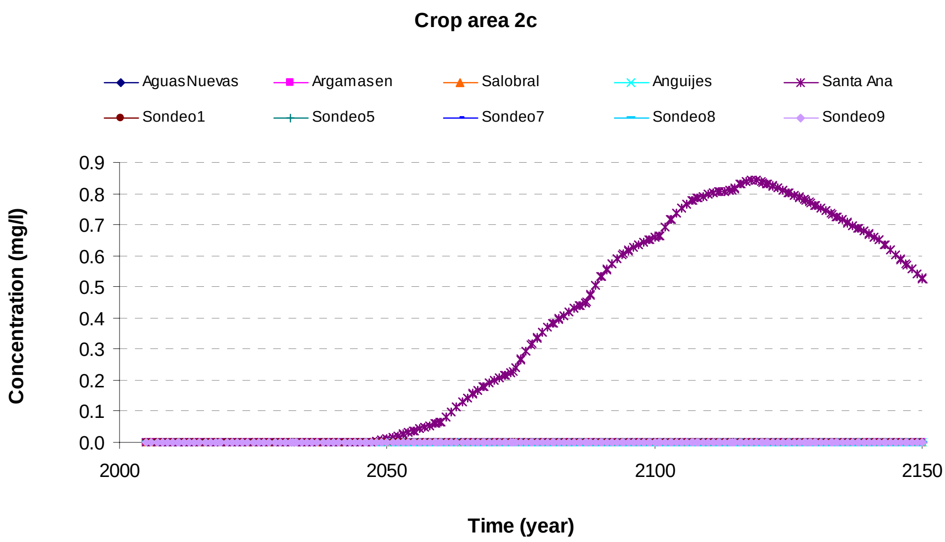

Figure C.4 Unitary concentration-time curves for crop area 2c

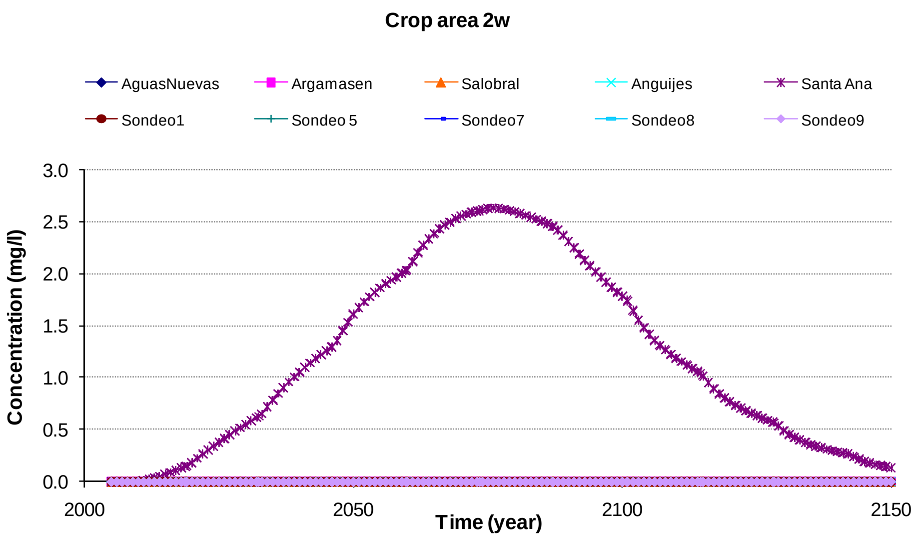

Figure C.5 Unitary concentration-time curves for crop area 2w

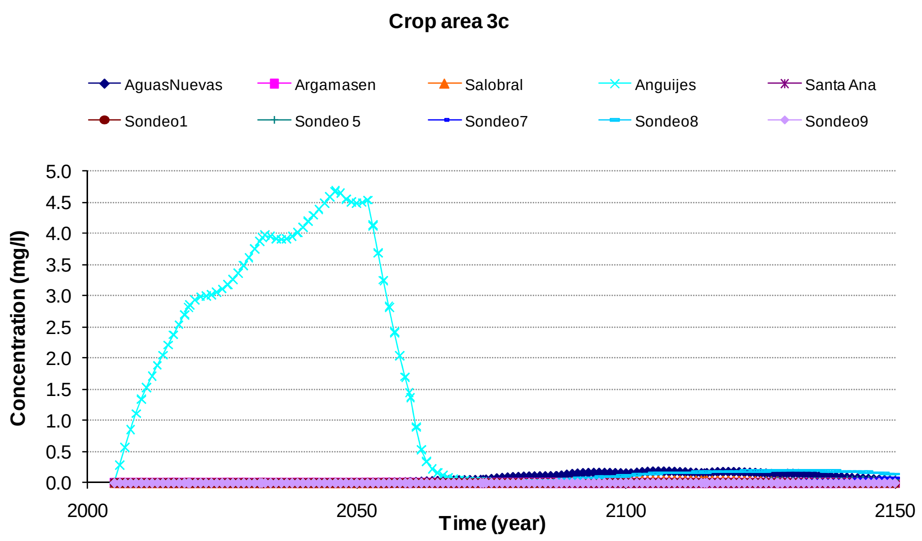

Figure C.6 Unitary concentration-time curves for crop area 3c

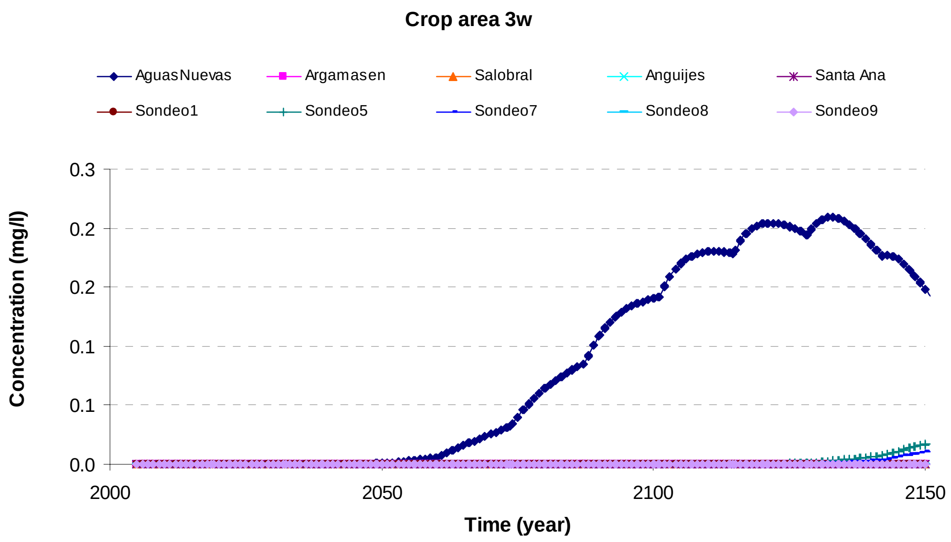

Figure C.7 Unitary concentration-time curves for crop area 3w

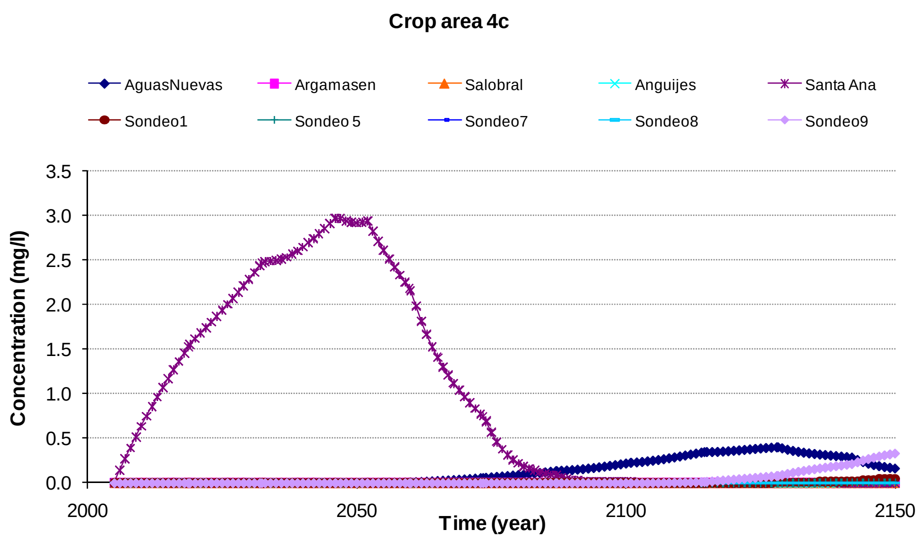

Figure C.8 Unitary concentration-time curves for crop area 4c

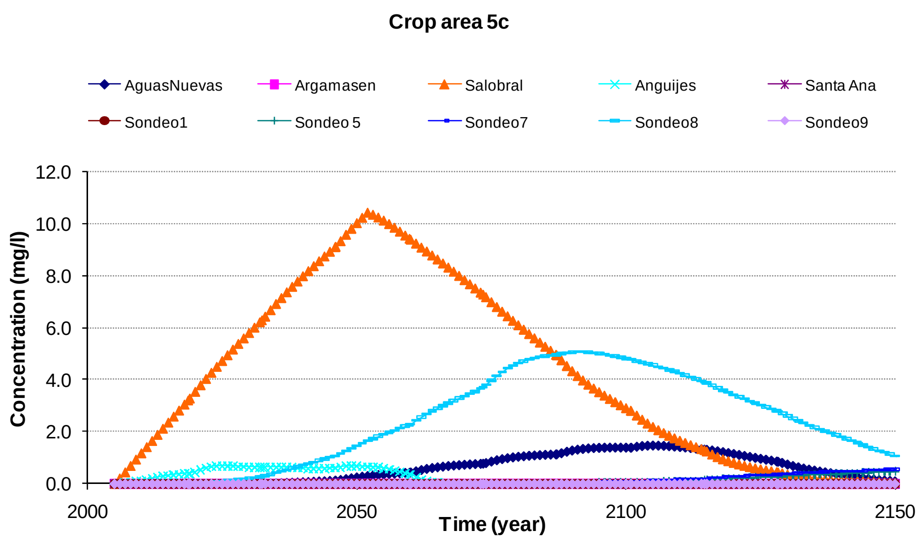

Figure C.9 Unitary concentration-time curves for crop area 5c

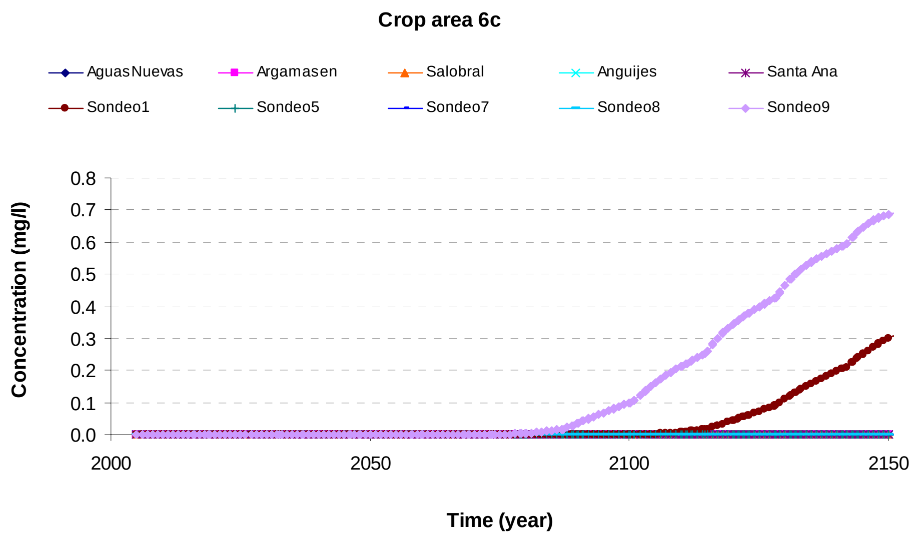

Figure C.10 Unitary concentration-time curves for crop area 6c

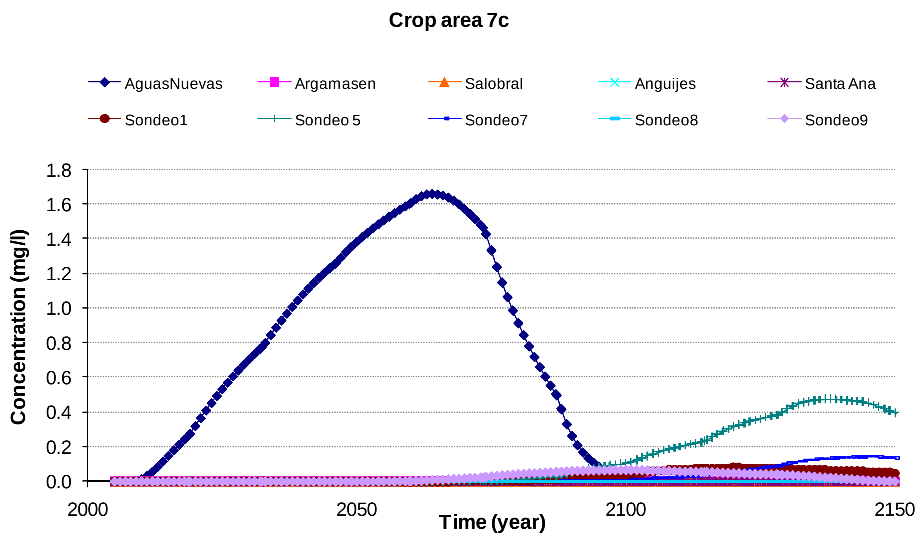

Figure C.11 Unitary concentration-time curves for crop area 7c

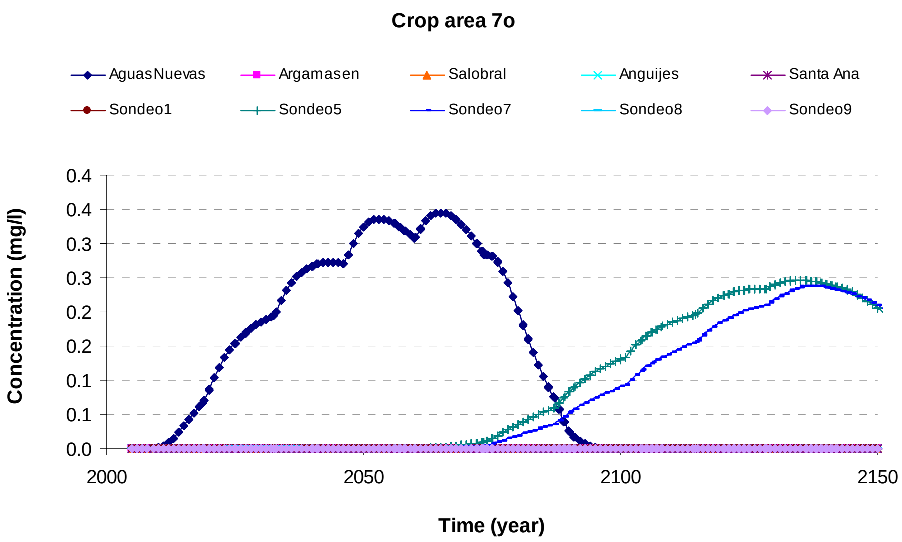

Figure C.12 Unitary concentration-time curves for crop area 7o

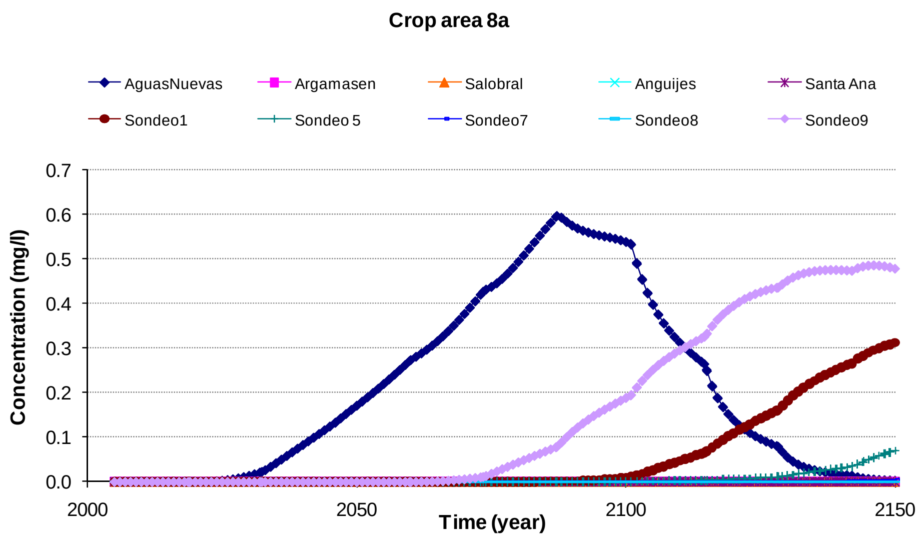

Figure C.13 Unitary concentration-time curves for crop area 8a

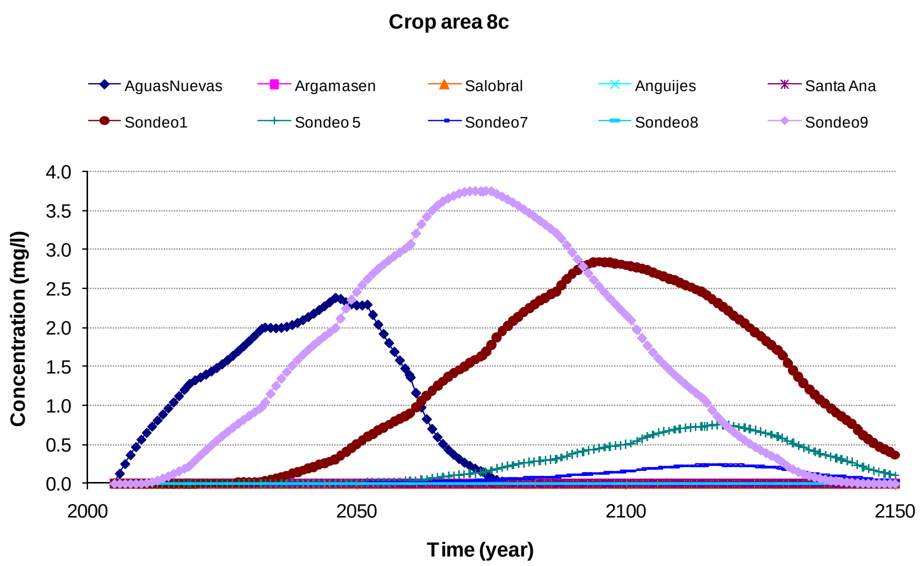

Figure C.14 Unitary concentration-time curves for crop area 8c

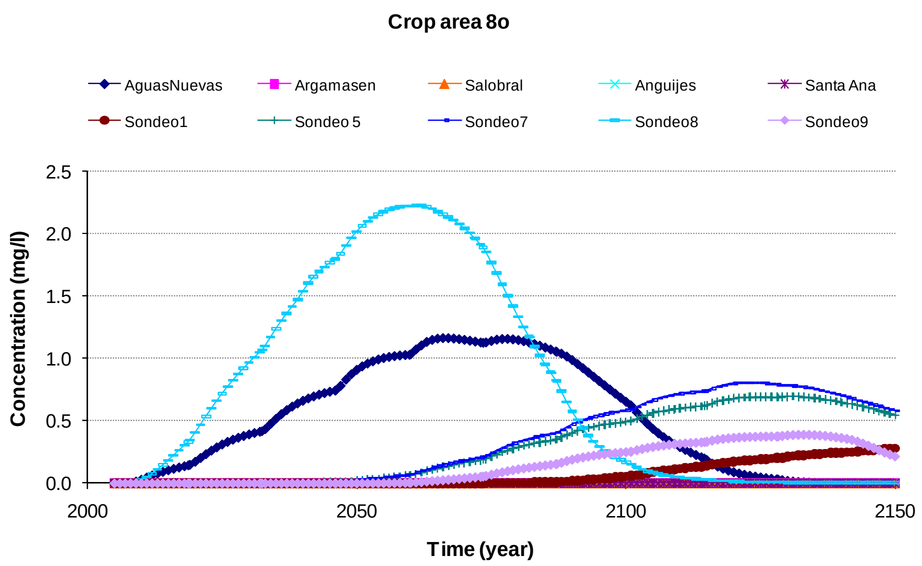

Figure C.15 Unitary concentration-time curves for crop area 8o

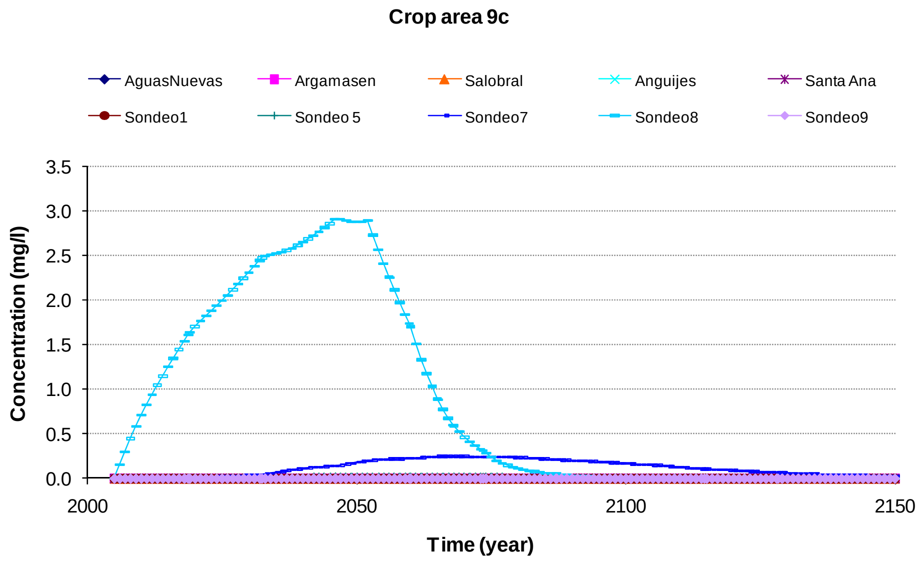

Figure C.16 Unitary concentration-time curves for crop area 9c

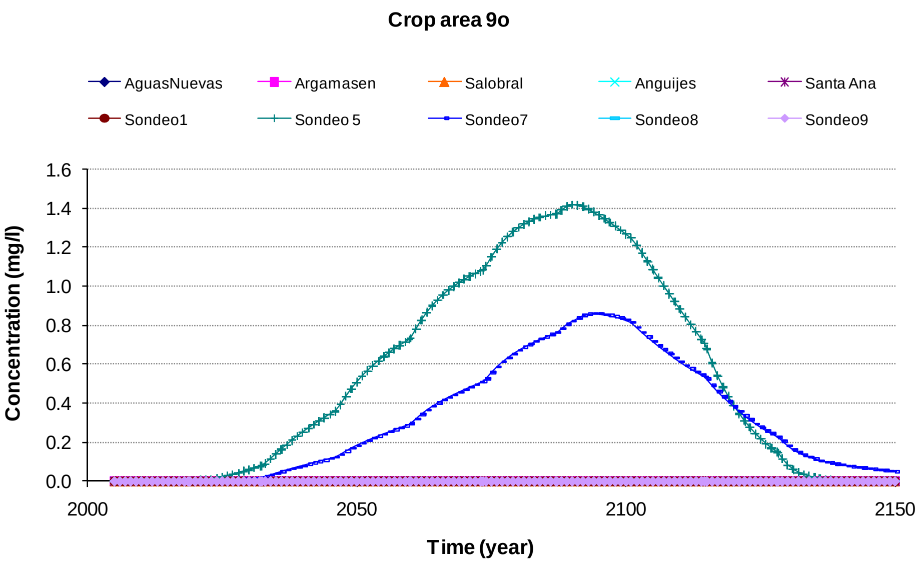

Figure C.17 Unitary concentration-time curves for crop area 9o

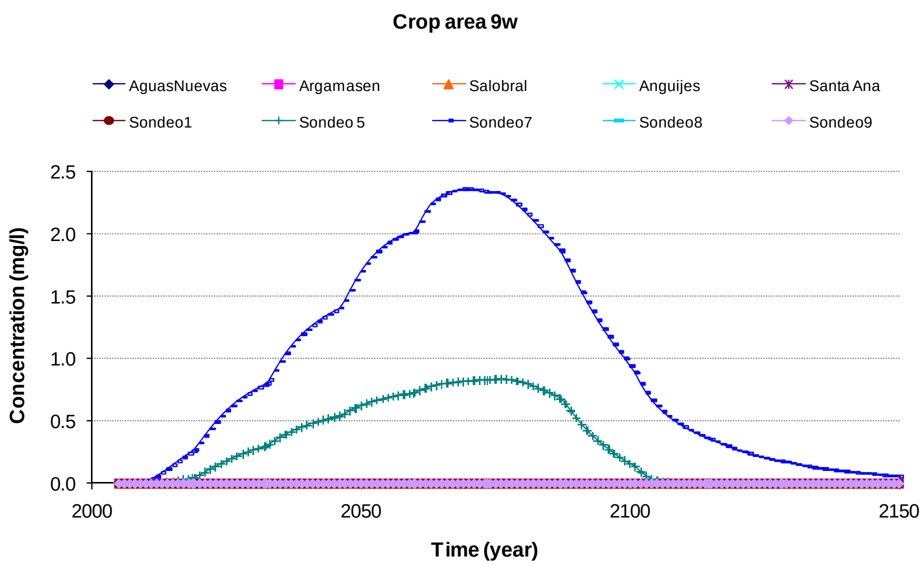

Figure C.18 Unitary concentration-time curves for crop area 9w

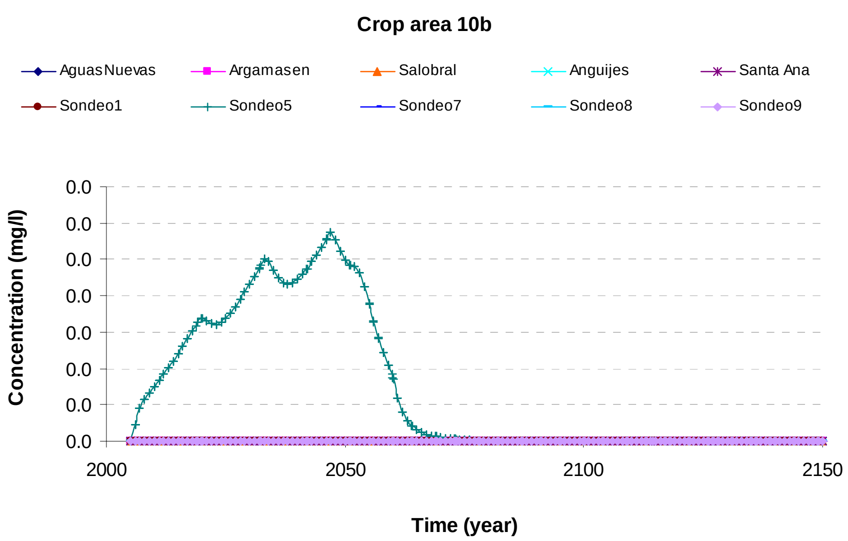

Figure C.19 Unitary concentration-time curves for crop area 10b

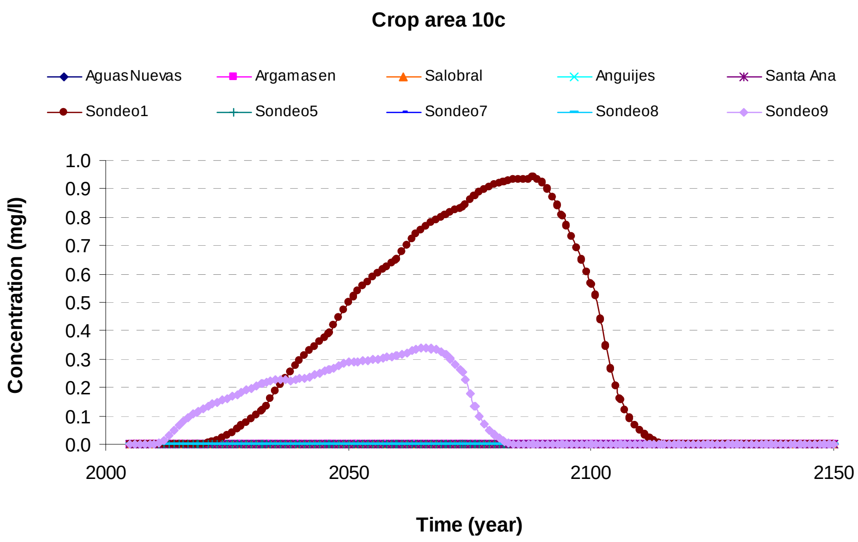

Figure C.20 Unitary concentration-time curves for crop area 10c

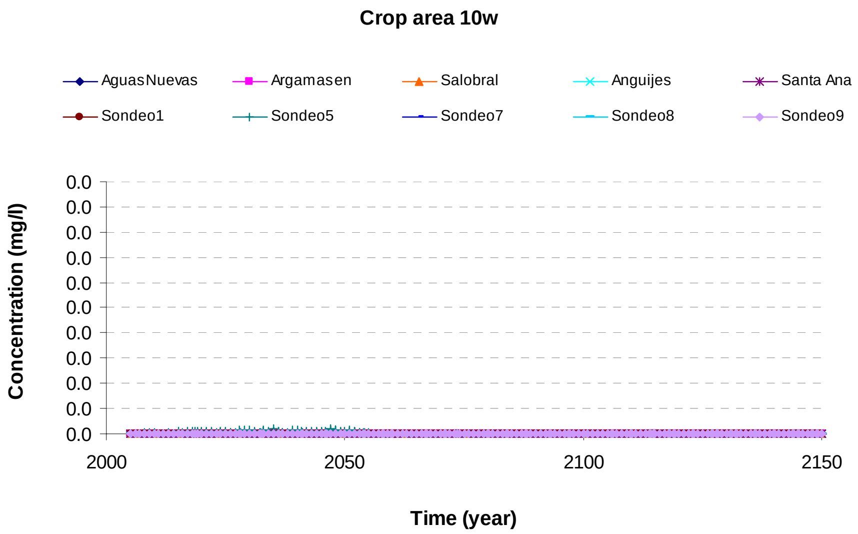

Figure C.21 Unitary concentration-time curves for crop area 10w

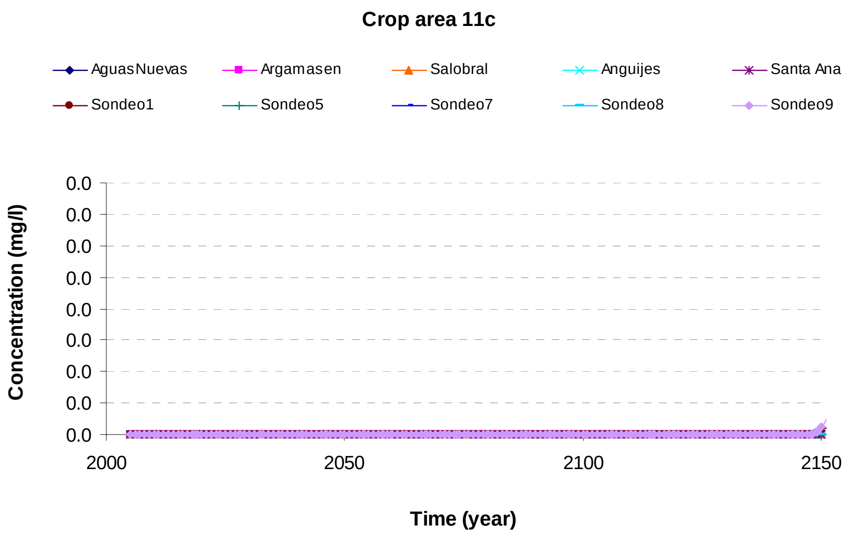

Figure C.22 Unitary concentration-time curves for crop area 11c

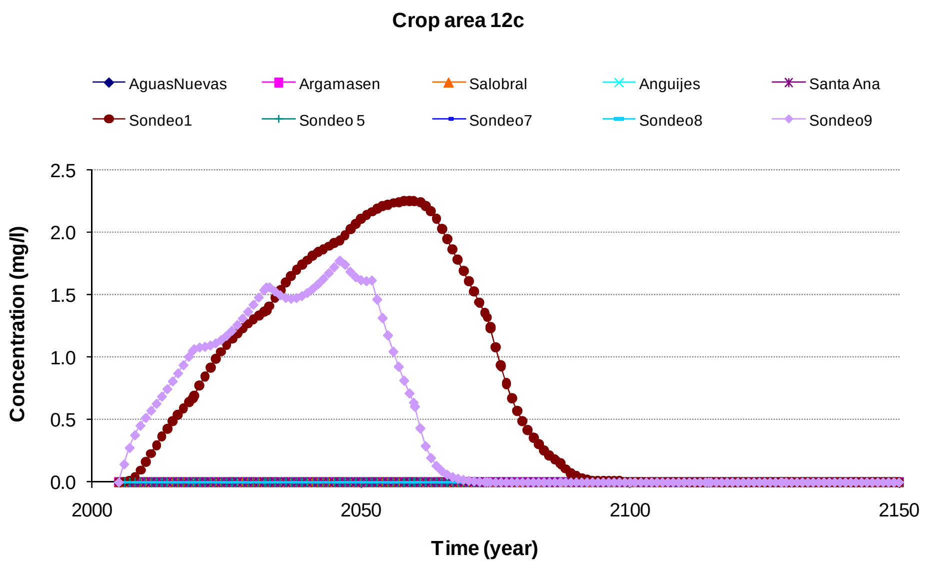

Figure C.23 Unitary concentration-time curves for crop area 12c

Appendix D. Farming costs. El Salobral-Los Llanos case study.

		Wheat	Corn	Barley	Alfalfa	Onion
Crop Yield	kg/ha	6501	13831	6034	15543	73295
Irrigation	m3/ha	2600	6600	3000	9000	6500
Crop price	€/kg	0.136	0.142	0.115	0.138	0.7
Groundwater level depth	m3/ha	100	100	100	100	100
Irrigation system pressure	kg/cm^2	5	5	5	5	5
Pumping efficiency	kWh/m^3	0.8176	0.8176	0.8176	0.8176	0.8176
Power	kW/ha	3	3	3	3	3
Power price	€/kW	7.78	7.78	7.78	7.78	7.78
Price of energy	€/kWh	0.05644	0.05644	0.05644	0.05644	0.05644
Gross production	€/ha	884.1	1964.0	693.9	2145.0	51306.6
Subsidy	€/kg	0.092	0.031	0.091	0.000	0.000
Subsidy	€/ha	598.1	424.8	552.0	0.0	0.0
Total income	**€/ha**	**1482.1**	**2388.8**	**1245.9**	**2145.0**	**51306.6**
Plants and seeds	€/kg	0.016	0.008	0.015	0.001	0.008
Fertilizer	€/kg	0.019	0.003	0.020	0.008	0.003
Phytosanitary	€/kg	0.005	0.001	0.004	0.004	0.001
Other products	€/kg	0.000	0.004	0.000	0.000	0.004
Subtotal	€/kg	0.040	0.016	0.039	0.013	0.016
Subtotal	**€/ha**	**262.2**	**224.7**	**237.4**	**206.1**	**1190.7**
Energy need	kWh/ha	2'125.8	5'396.2	2'452.8	7'358.4	5'314.4
Power cost	€/ha	23.3	23.3	23.3	23.3	23.3
Energy cost	€/ha	120.0	304.6	138.4	415.3	299.9
Tax	€/ha	7.0	8.0	9.0	10.0	11.0
IVA (16%)	€/ha	24.1	53.7	27.3	71.8	53.5
SubTotal	€/ha	174.4	389.6	198.1	520.4	387.8
Maintenance	€/ha	18.0	18.0	18.0	18.0	18.0
Cost	**€/ha**	**192.4**	**407.6**	**216.1**	**538.4**	**405.8**
Work	€/Kg	0.01078	0.00340	0.01177	0.00952	0.00000
Fuel	€/Kg	0.00486	0.00114	0.00477	0.00176	0.00039
Maintenance	€/Kg	0.00273	0.00076	0.00273	0.00156	0.00019
Total machinery costs	€/Kg	0.01837	0.00530	0.01926	0.01283	0.00058
Total machinery costs	**€/ha**	**119.4**	**73.4**	**116.2**	**199.4**	**42.6**
Labor	**€/ha**	**32.6**	**52.6**	**27.4**	**47.2**	**1128.7**
Direct costs	**€/ha**	**606.6**	**758.3**	**569.7**	**943.9**	**1639.1**
Indirect costs	**€/ha**	**44.2**	**98.2**	**34.7**	**107.2**	**2565.3**
Total costs	**€/ha**	**650.8**	**856.5**	**604.4**	**1051.1**	**4204.4**

*Source Spanish Ministry of Environment and Ministry of Agriculture. 2004 data

To infinity and beyond!

B.L.