Hydrus-1D as a tool to understand contamination of an aquifer:

A case study in the Central Valley of Cochabamba

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Theo Nyberg

Abstract

In water resource management, it is of importance to be able to predict how different activities might contaminate aquifers. For this kind of application, numerical modelling of water and solute transport can be a useful tool. The purpose of this study was to investigate if one-dimensional numerical modelling (Hydrus-1D) of water in the unsaturated zone of the subsoil is useful to assess the transport of contaminants from the soil surface to aquifer. More specifically, the goal set up was to develop a conceptual model of the hydrogeological and hydrogeochemical situation at the site of a deep well (Tiquipaya) located in the Central Valley of Cochabamba, Bolivia, and to adjust this to a Hydrus-1D model.

In the study, the specific case that was considered was the subsoil of an agricultural field where onion is cultivated. The contaminant of interest was nitrate, which entered the subsoil through the application of urea-fertilizers dissolved in water from flood irrigation. The model attempted to capture the transport of water and solute through the unsaturated zone down to the groundwater level.

The goal of the study was reached in the sense that a conceptual model was develop and adjusted to Hydrus-1D. However, it required several major assumptions and simplifications regarding the site-specific conditions and the input parameters associated with them. In particular, parameters related to soil characteristics were derived from a simple description, despite being considered as important for the simulation results.

The limitations associated with the simplifications and assumptions made while setting up the model meant that the specific results of the simulations are of limited use. However, in line with the purpose of the study, they were considered plausible enough for deeming the model to have a potential for being used in water resource management. Thus, the main conclusion of the study was that numerical modelling (Hydrus-1D) is suitable for assessing groundwater contamination, but that further studies must be performed to improve the accuracy of the model for it to be able to provide useful results.

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1. Introduction

As the perhaps most basic but vital resource we have, across the globe water is increasingly attracting attention from both academia and authorities as a resource that must be protected. Drastic population increases over the last century, coming with both an increase in demand but also with increased contamination in existing water resources has put the water scarcity on the agenda of most authorities.

In the Central Valley of Cochabamba, Bolivia, the semi-arid climate has meant that surface water is insufficient to meet the demand from the population. Instead, groundwater has been the major source of supply, where the alluvial fans have served as important aquifers. A drastic increase in population in the last decades has meant that the demand for water has increased significantly, putting more pressure on existing water resources. Meanwhile, the population increase in combination with an intensified use of fertilizers and pesticides for agriculture, has meant that these reservoirs are now more vulnerable to contamination, with the risk of making them unsuitable for human needs (Renner & Velasco, 2000).

In order to be able to protect these reservoirs it is important to understand how and at what rate they are affected by infiltrating contaminants. One way to increase this understanding is to make use of numerical modelling to estimate how solute transport takes place through the soil layers. However, modelling is a tool which usefulness and credibility could vary. It is important that the model is calibrated to the specific site, with more detailed information giving a higher credibility of the model. Also, it could be beneficial to be able to compare the results of the model with real measured data, in order to validate the accuracy of the model. Unfortunately, the situation in Bolivia is often characterized by a lack of data, and studies of the groundwater situation are not abundant. This puts a limit on the usefulness of modelling results.

For this reason, this study aims to investigate if one-dimensional modelling of solute transport in the unsaturated and saturated zone can be useful to predict, prevent and mitigate groundwater contamination. If the model proves to be useful, it could be a basis for further research, in which it could be complemented by field surveys, both to provide better input data, but also in order to be able to validate the results.

1.1. Purpose and research questions

The purpose of this study was to investigate if one-dimensional numerical modelling (Hydrus-1D) of water in the unsaturated zone of the subsoil is useful to assess the transport of contaminants from the soil surface to aquifers. Therefore, the goal of the study was to develop a conceptual model of the hydrogeological and hydrogeochemical situation at Tiquipaya and to adjust this to a Hydrus-1D model. To reach this goal, the following sub goals were set up:

I. Collect available information about the hydrogeological and hydrogeochemical conditions

II. Assess how potential contaminants (nitrate) might interfere with the groundwater through the use of fertilizers and flood irrigation

III. Acquire an understanding of what data is required in order to erect a sufficiently accurate Hydrus-1D model

IV. Adjust the conceptual model and combine it with relevant data into a Hydrus-1D model

V. Assess the plausibility of the results from the Hydrus-1D simulation

2. Background

2.1. General description of area

The study area is located in the Central Valley of Cochabamba, Bolivia, (see fig. 1) which is part of the sub-Andean valleys. An arid to semi-arid climate characterizes the region, with moderate rainfalls and high evaporation rates (Renner & Velasco, 2000). Rapid population growth has taken place over the last century, and is still ongoing, where the 2012 population of 1 536 145 citizens in the metropolitan area was projected to almost double until 2036 (MMAyA, 2014). This has led to a drastic increase in water use, mainly needed for irrigation and human consumption (MMAyA, 2014). In combination with the dry climate, this has meant that surface waters have been unable to satisfy the demands for water, which is why the groundwater resources have become of great importance. 2012 the number of wells in the valley exceeded 1500 (MMAyA, 2014) and today it might be more than 2000. A large part of the valley is used for agriculture, where onions, potatoes, corn, alfalfa and beans are the most important crops (MMAyA, 2014; Renner & Velasco, 2000). All of these except onions and alfalfa are cultivated in a determined season once per year. The agricultural activities are an important factor for water management both because of the demand for water and for the contamination risk it poses.

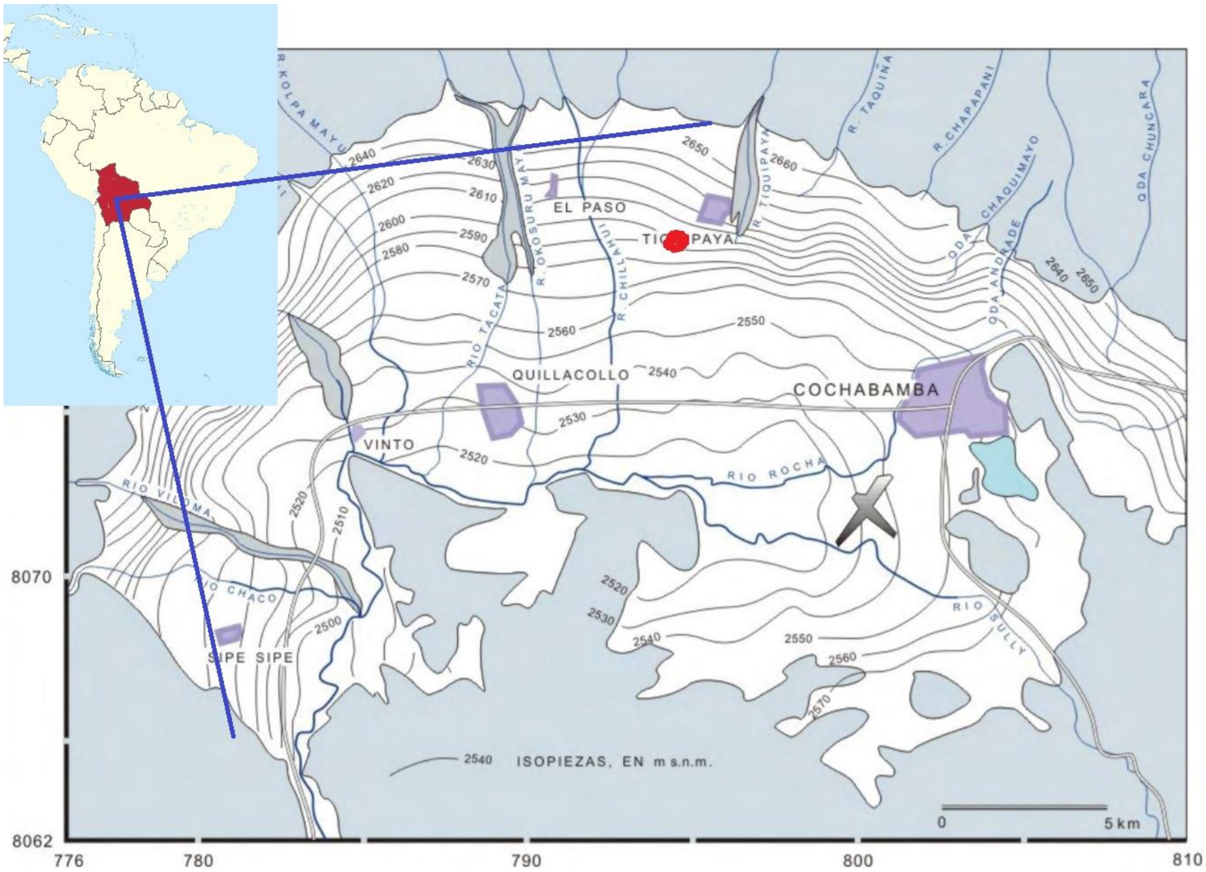


Figure 1. Map of Bolivia in South America and piezometric map of the Central Valley of Cochabamba, with the approximate location of the Tiquipaya well marked with a red dot. Map taken from Wikimedia Commons and piezometric map adapted from Fig. 32 in Renner and Velasco (2000).

2.2. Geology

The basin has for long periods of time been occupied by a lake, the extent of which has varied over several cycles. For this reason the quaternary sediments of the basin consists of an interfingering of lacustrine and alluvial materials. The alluvial layers, having been formed when the withdrawal of the lake has exposed flat plains, mainly consist of coarse-grained materials transported down in rivers along the steep mountainsides. At the foot of the mountains, where the flatter gradient causes the river to flow slower, deposited coarse materials have formed alluvial fans. The lacustrine layers, on the other hand, have been formed at times when the lake has been more extensive. These layers are instead dominated by finer materials deposited in the more still waters of the lake (Renner & Velasco, 2000).

The location for the modelling in this study is the site of a deep well, Tiquipaya, in the northern part of the Central Valley of Cochabamba. A lithological profile of the site can be seen in figure 2 from which three different lithological units can be identified above what is termed the deep aquifer (starting at a depth 265 m.b.s). With help of the piezometric map from Renner and Velasco (fig. 1) and the fact that the ground level is located at an altitude of 2670 meters (Renner & Velasco, 2000) one can conclude that the groundwater level of this unconfined aquifer is located approximately 80 meters below the surface, but with the clay layer starting at 240 meters depth likely to form a confining layer between the two aquifers. This also means that percolation of water down to the top unconfined aquifer takes place in the unsaturated zone of the top layer of blocks, gravel and sand in fig. 2.

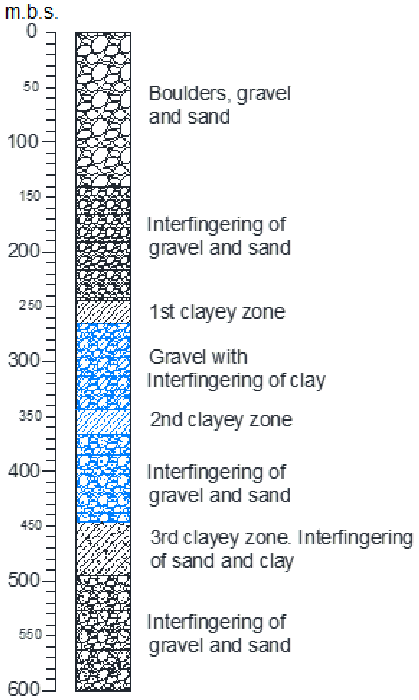


Figure 2. Lithological profile of the perforation Tiquipaya. Figure adapted from Fig. 28 in Renner and Velasco (2000).

2.3. Water resources

Water supply in the area comes from both subterranean and superficial sources. The groundwater resources - which as per 2012 provided 65% of the supply in the metropolitan area (MMAyA, 2014) - are mainly found in the geological units of the alluvial fans (Renner & Velasco, 2000). The superficial sources are both lake reservoirs found in the Tunari range, north of the valley, but also the rivers that cross the valley, where Rocha River and Tamborada River are the two main ones. Apart from these existing sources, the so-called Misicuni dam was built in the first decennia of the 21st century as a multipurpose dam to divert water from Misicuni River for various water uses but also in order to generate electricity from a hydroelectric power plant. To this date, however, the channels connecting it to Cochabamba have not been finalized, meaning that it does not provide any water at this point (but is estimated to have a potential of 3200 liters per second (MMAyA, 2014)).

Due to the arid climate of the region, freshwater is a scarce resource, with the supply only covering 54% of the demand in 2012 (MMAyA, 2014). Furthermore, increased anthropogenic impact has meant that the resources that exist are often of poor quality. This is the case for some of the major rivers, where pollution is a major issue (Jacobson and Sekizovic, 2019). In some regions the shortage of clean water has even forced the agricultural sector to make use of alternative sources for water, such as treated or untreated sewage water (Zabalaga et al., 2007). In this context, groundwater is a precious resource. However, even this resource is at risk, where both overexploitation and contamination threaten future security of supply, which is why the protection of aquifers is a vital issue.

2.4. Contamination risks

Vulnerable areas

In order to be able to predict and prevent contamination of aquifers it is important to identify which areas that are vulnerable to contamination. In the case of groundwater, contamination can either come from the spreading of existing contaminated zones (e.g. saline zones) or from water that infiltrates at the soil surface and percolates down to the groundwater. In this study it is mainly the latter type that is of interest, and in order to categorize vulnerable areas it is necessary to identify where groundwater recharge takes place. In the Central Valley of Cochabamba aquifer recharge mainly takes place in the alluvial cones, which are generally constituted of coarse-grained materials (Renner & Velasco, 2000). This percolation mainly comes from rivers descending the mountains, but also, to a probably lesser extent, from precipitation and irrigation water (Renner & Velasco, 2000). A recent study on the geographically proximate Punata alluvial fan demonstrated that vertical recharge from rainfall and irrigation waters is likely of minor importance in that area (Gonzales et al., 2018). However, the alluvial cones are the main recharge areas, and are thus important to consider when protecting groundwater resources.

Sources

The main sources of contamination in the basin are agriculture, industrial effluents and human waste. In the case of agriculture the risk comes both from the use of fertilizers/pesticides but also - with the increasing contamination of rivers as well as the reuse of wastewater - from the general quality of irrigation water.

Major contaminants

In the Central Valley of Cochabamba the major contamination is occurring in the Rocha River, where metals, organics and other pollutants may be found. However, in the agricultural lands, nitrate derived from fertilizers is likely to be the most important contaminant. This is also the compound that will be the focus of this study, which is why a more elaborated description on how it behaves is needed.

Nitrate chain

Nitrogen (N) is an essential element for plants and is often introduced as urea, $CO(NH_2)_2$, in fertilizers. Dissolved in water, urea-N is transformed through the so-called nitrogen chain (fig. 3). This starts with the hydrolysis of urea to ammonia, NH_3 (dissolved to ammonium, NH_4^+). Organic nitrogen in the soil can also be microbially and enzymatically degraded to form inorganic ammonium. This process is known as mineralization. Ammonium can form nitrate through the process of nitrification. The middle species nitrite is often neglected due to the much faster reaction from nitrite to nitrate (Hanson et al., 2006). The nitrate, in turn, can be denitrified to nitrogen gas, N_2, or nitrogen oxide, N_2O. Apart from these transformations, ammonium can also be volatilized as ammonia as well as adsorb to soil particles. Ammonium and nitrate are the two forms of nitrogen that are readily available for plant uptake.

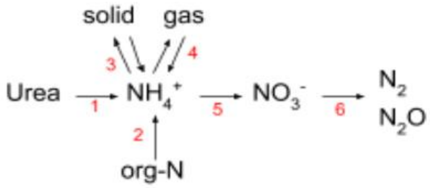


Figure 3. Nitrogen chain, including processes of urea hydrolysis (1), mineralization (2), adsorption (3) and volatilization (4) of ammonium, nitrification (5) and denitrification (6).

3. Model

3.1. Model description

The model description that follows here is based on the technical manual for Hydrus-1D provided on the website of PC-Progress (Šimůnek et al., 2012).

Hydrus-1D is a modelling program used to model water flow and solute transport in unsaturated, partially saturated or saturated porous media. It uses Galerkin-type linear finite element schemes to numerically solve the Richard's equation (eq.1) for saturated-unsaturated water flow and the Fickian-based advection-dispersion equation (eq. 2) for solute transport.

The modelling of water flow, as mentioned before, is based on the Richard's equation which is a partial differential equation describing water movement in unsaturated soils. In its transient, one-dimensional form it looks below:

$$\frac{\delta\theta}{\delta t} = \frac{\delta}{\delta z} \cdot [K(\theta) \cdot (\frac{\delta h}{\delta z} + 1)] - S \tag{1}$$

where θ is the volumetric soil water content (-), h is the pressure head (L), t is the time (T), z is the vertical space coordinate, K is the hydraulic conductivity (L T^{-1}) and $S$is an optional sink term that accounts for root water uptake (T^{-1}).

Unsaturated soil hydraulic parameters are determined using van Genuchten (1980), Brooks and Corey (1964) and modified van Genuchten type analytical functions. These describe functional relationships between saturation, pressure and permeabilities of unsaturated porous media. The van Genuchten equation (eq. 2 and 3) explains why the hydraulic conductivity, K, in Richard's equation (eq.1) is a function of water content, θ, and in turn depth in column, h.

$$S_e(h) = \frac{\theta(h)-\theta_r}{\theta_s-\theta_r} = \frac{1}{(1+|\alpha h|^{\eta})^m} \tag{2}$$

$$K(h) = K_s S_e^l [1-(1-S_e^{1/m})^m]^2 \tag{3}$$

where $S_e$is the effective water content (-), h is the pressure head (L), θ is the water content (-), r and s indicate saturated and residual values, respectively, K is the hydraulic conductivity (L T^{-1}) and α, η, m and l are empirical parameters.

In Hydrus-1D, root water and nutrient uptake is modelled using a macroscopic approach. This means that effects of root geometry and flow pathways around roots are neglected. Instead, root water and nutrient uptake are formulated using a single sink term in the mass balance equations. Furthermore, the models provide the opportunity of considering solute stress, which is the effect salinity could have on root uptake. Also, solute uptake is divided into an active and passive part, where the passive part is calculated by multiplying root water uptake with the solute concentration.

Flow and transport can occur in vertical, horizontal or inclined directions and can deal with nonuniform soils. Boundary conditions can be atmospherically controlled, prescribed by (constant or time-varying) head and flux or they could be free drainage boundaries.

The solute transport considers advection-dispersion transport in the liquid phase and diffusion in the gaseous phase. It is based on the Fickian advection-dispersion model which is displayed in its most simple form in eq. 4. The first term represents advective transport, the second term dispersive transport and the third one is the reaction term.

$$\frac{\delta C}{\delta t} = -v\frac{\delta C}{\delta x} + D_L\frac{\delta^2 C}{\delta x^2} - \frac{\delta q}{\delta t} \tag{4}$$

where C is the solute concentration (M L^{-3}), v is the pore water flow velocity (L T^{-1}), x is distance (L), $D_L$is the hydrodynamic dispersion coefficient (L T^{-1}), t is time (T) and q (M L^{-3}) is the concentration in the solid phase.

It includes provision of nonlinear nonequilibrium reactions between solid and liquid phases, linear equilibrium reactions between liquid and gaseous phases, zero-order chemical production and two first-order degradation reactions. Also, physical nonequilibrium solute transport can be considered by using dual-porosity models. In such cases the porosity systems are divided into mobile and immobile parts between which mass transfer can occur through diffusion.

3.1.1. Case-specific model details

In this study the following processes of N-transformation were considered: (1) hydrolysis of urea to ammonium; (2) mineralization of organic N to ammonium; (3) adsorption of ammonium; (4) ammonia volatilization; (5) nitrification of ammonium to nitrate; (6) denitrification of nitrate; (7) root uptake of ammonium and nitrate. Reactions 1, 5 and 6 are all considered as first-order processes (Hanson et al. 2006) while reaction 2 is considered a zero-order reaction. Reaction 3 and 4 are equilibrium reactions.

Below can be found the more comprehensive partial differential equations describing one-dimensional transport of N involved in sequential first-order decay chain reactions during transient water flow in a variably saturated medium:

$$\frac{\delta\theta C_1}{\delta t} = \frac{\delta}{\delta z}\left(\theta D_1^w\frac{\delta C_1}{\delta z}\right) - \frac{\delta q C_1}{\delta z} - \mu'_{w,1}\theta C_1 \tag{5}$$

$$\begin{aligned}\frac{\delta\theta C_2}{\delta t} + \frac{\delta\rho s_2}{\delta t} + \frac{\delta a_v g_2}{\delta t} &= \frac{\delta}{\delta z}\left(\theta D_2^w\frac{\delta C_2}{\delta z}\right) + \frac{\delta}{\delta z}\left(a_v D_2^g\frac{\delta g_2}{\delta z}\right) - \frac{\delta q C_2}{\delta z}\\ &\quad -\mu'_{w,2}\theta C_2 + \mu'_{w,1}\theta C_1 + \gamma_{s,2}\rho - r_{a,2}\end{aligned} \tag{6}$$

$$\frac{\delta\theta C_3}{\delta t} = \frac{\delta}{\delta z}\left(\theta D_3^w\frac{\delta C_3}{\delta z}\right) - \frac{\delta q C_3}{\delta z} - \mu_{w,3}\theta C_3 + \mu'_{w,2}\theta C_2 - r_{a,3} \tag{7}$$

where C is the concentration of solute in the liquid phase (M L^{-3}), S is the concentration of solute in the solid phase (-), g is the concentration of solute in the gas phase (M L^{-3}), θ is the volumetric water content (-), ρ is the dry bulk density (M L^{-3}), q is the volumetric flux density (L T^{-1}), μ_w is the first-order rate constant for solute in the liquid phase (T^{-1}), μ'_w is also a first-order rate constant, but one which provides connections between individual chain species, γ_s is a zero-order rate constant in the solid phase (T^{-1}), r_a represents root nutrient uptake (M L^{-1} T^{-1}), D^w is the dispersion coefficient (M^2 T^{-1}) for the liquid phase and D^g is the diffusion coefficient (L^2 T^{-1}) for the gas phase. The subscripts 1, 2 and 3 in these equations represent urea, ammonium and nitrate respectively.

Ammonium is the only of the species for which adsorption is considered, and this process is treated as an instantaneous reaction between the soil solution and the exchange sites of the soil matrix (equilibrium model). The relation between S_2 and C_2 is captured by the distribution coefficient, $K_{d,2}$, found in the linear equation 8:

$$S_2 = K_{d,2} C_2 \tag{8}$$

$K_{d,2}$ thus represents the coefficient that describes the linear relationship between S_2 and C_2.

3.2. Conceptual model

A conceptual model has been developed in order to understand and describe the hydrogeological and hydrogeochemical situation at the site. This then forms the basis of all the settings and assumptions of the Hydrus-1D model. The conceptual model is visualized in figure 4.

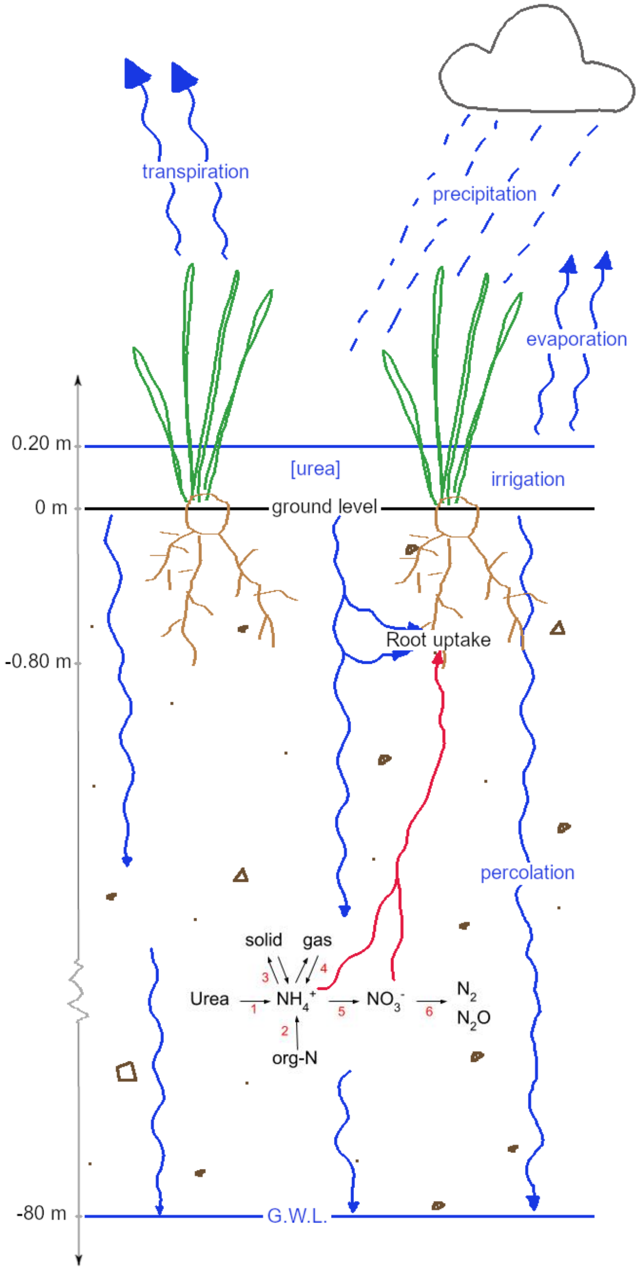


Figure 4. Conceptual model that was set up in the study.

The geological characteristics of the profile are simplified by the fact that the groundwater level (located at 80 meters depth) is situated above the second lithological layer, which starts at approximately 140 meters depth. This means that the top lithological layer makes up the whole unsaturated zone, which is where this study focuses. Since this layer consists of boulders, gravel and sand it could be considered to have a considerable hydraulic conductivity.

Water that enters the soil profile comes both from precipitation and irrigation, but they are not differentiated in the model. When irrigation takes places, it is added upon the natural precipitation. The soil is irrigated through flood irrigation, meaning that a channel is opened to let the soil be flooded. Since this is not an instantaneous process, the flooding is assumed to be distributed over 20 hours each irrigation day. The irrigation frequency is every fourth day during the first two months of the cropping season and once a week during the third (and last) month.

Some of the added water is lost through evaporation and through transpiration after root water uptake. Root uptake is simplified by assuming that no root growth takes place. Instead the roots instantly penetrate to a depth of 80 cm once planted, and then keeps the same size and uptake characteristics for the whole cropping period.

Water that is not lost through evaporation or root uptake percolates through the unsaturated soil profile until it eventually reaches the groundwater level. The water content of the soil has a minimum level (referred to as the residual water content, θ_r) for which further increases in the soil's suction result in only marginal changes in water content. Water leaves the soil profile through the bottom boundary which represents the groundwater level.

At times when irrigation takes place, nitrogen is assumed to infiltrate the soil surface in the form of urea dissolved in the water. While this water percolates down through the initially unsaturated profile, nitrogen is transformed through the nitrogen chain (fig. 3).

This chain includes hydrolysis of urea to ammonia, mineralization of org-N to ammonium, nitrification of ammonium to nitrate and denitrification of nitrate to nitrogen gas (which leaves the system). Ammonium is also assumed to be adsorbing to soil particles as well as establishing an equilibrium with its gas phase through volatilization. Both ammonium and nitrate can leave the system through root nutrient uptake, since both these forms of nitrogen are accessible to plants.

3.3. Model setup

In order to develop a Hydrus-1D model there are various different settings to choose from. A full list of all model choices, input parameters and their sources (where exists) can be found in the Appendix A1. However, some of the assumptions are of extra relevance and will thus be explained and motivated here.

3.3.1. Pre-simulation

One such choice concerns the duration of the simulation. Since no information on the soil's water content was at hand, pre-simulation was done in order to acquire a realistic water content. This pre-simulation was almost eleven months long and preceded the three-month period during which fertilization took place and the onion was growing (the "cropping period", starting after 7769 hours). A major difference between the pre-simulation period and the cropping period was that the pre-simulation was run without irrigation, fertilization and crops. Instead, natural precipitation and other atmospheric conditions were governing the hydraulic conditions at the end of the pre-simulation and the start of the cropping period.

3.3.2. Sub models

Other important assumptions concern the choices of different sub models that were made when setting up the model in Hydrus-1D. One assumption is that the hydraulic model is set to be a single porosity model (van Genuchten-Mualem model), instead of dual-porosity. This assumes that there are no major differences in hydraulic permeability, meaning that only mobile flow regions exist.

The solute transport model is set to an equilibrium model, which indicates that solute partitioning between the liquid and solid phase is assumed to be instantaneous (i.e. not kinetically controlled). Thus, the adsorption is independent of residence time.

For the root uptake, only passive root nutrient uptake was considered. Thus there is no possibility for plants to compensate for reduced passive uptake. This is a typical assumption in this kind of studies, motivated by the complexity of the mechanisms and the yet undetermined relative magnitude of relevance (Hanson et al., 2006; Ravikumar et al., 2011; Ramos et al., 2012).

3.3.3. Input parameters

One very important simplification for the input parameters is that all soil hydraulic parameters have been set using the built-in Rosetta module of Hydrus-1D. It uses neural network prediction to provide values of residual water content, saturated water content, hydraulic conductivity etc. based on a weight percentage of sand/silt/clay of the material. Thus, these parameters were set by the Rosetta module, where the already simple input values (sand/silt/clay%) were based on the description of the material as “blocks, sand and gravel” (Renner & Velasco, 2000).

The reaction parameters, which, among other things, govern reaction rates for the different processes of the nitrogen chain, were taken from other similar studies. For instance, hydrolysis of urea ($\mu'_{w,1}$ in eq.5-6) was set to $0.38 day^{-1}$(Hanson et al., 2006), nitrification of ammonium ($\mu'_{w,2}$ in eq.6-7) to $0.2 day^{-1}$(Hanson et al., 2006) and denitrification ($\mu_{w,3}$in eq.7) to $0.04 day^{-1}$(Li et al., 2015).

Similarly to the soil hydraulic parameters, the parameters for root uptake were set from a built-in database. For the Feddes’ parameters this was assumed to be the parameters for onion at bulbing-time during the whole cropping period.

Furthermore, hysteresis is neglected, implying that neither the retention curve nor the hydraulic conductivity is affected by its history. On the contrary, it is only the present state that matters.

Dependences on temperature and water content for transport and reaction parameters was neglected, according to common practice (Chowdary et al., 2004; Hanson et al., 2006).

3.3.4. Boundary conditions

Water flow

For the water flow, boundary conditions were set to “atmospheric BC with surface layer” and “free drainage” at the top and bottom respectively. The top condition was set so to allow for the use of real meteorological data while also allowing for flooding to occur. The bottom condition was motivated by the long distance from soil surface to the groundwater level, which with a constant pressure head could have given inaccurate results.

Solute transport

In solute transport, the boundary condition at the top was set to “concentration flux BC”. This indicates that the concentration of incoming water is set as input data. The bottom boundary condition was set to “zero gradient” indicating that the concentration will not change over the last depth of the profile.

4. Results

4.1. Water flow

The focus of this study was the three-month cropping period during which fertilizer was added, but the background to the starting condition could be understood by looking at the conditions for the whole extended period. Figure 5 visualizes water content at four different depths during this extended period. Over the three-month cropping period, approximately 600 cm^3 of water infiltrated each cm^2 of soil (fig. 12 in Appendix A2).

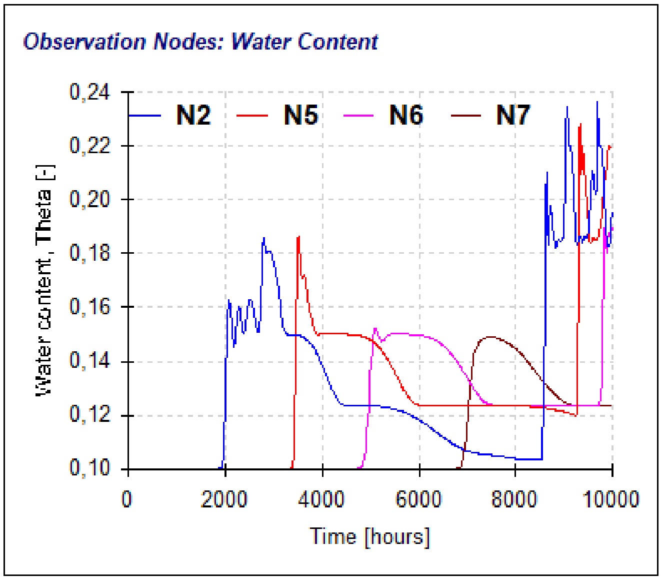
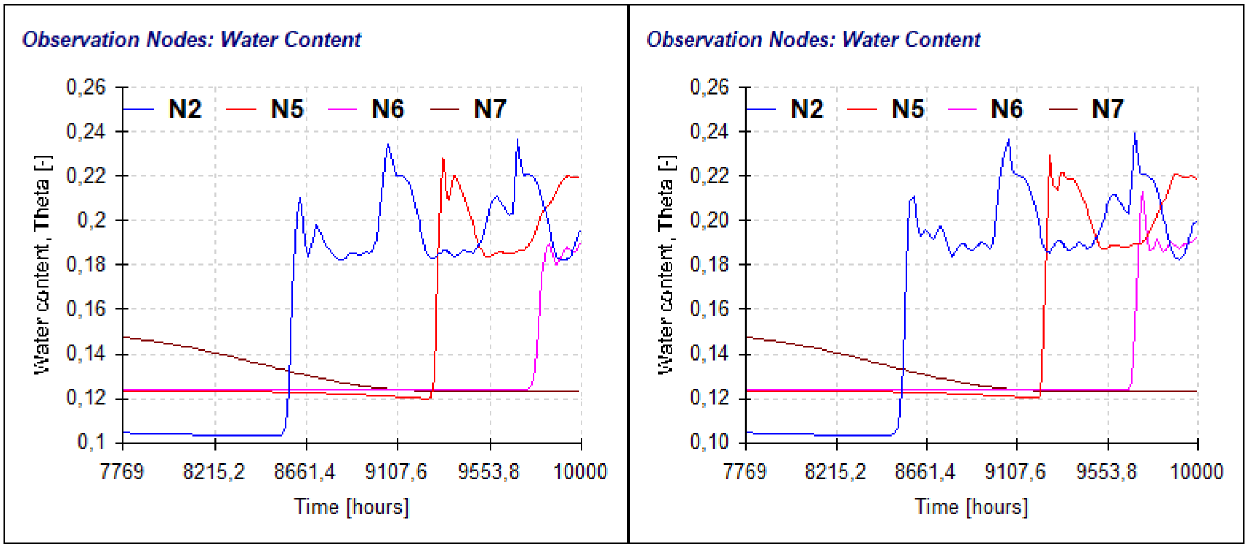


Figure 5. Water contents for the whole simulation period (pre + cropping) at observation nodes at four different depths: N2=20 m.b.s., N5=40 m.b.s., N6= 60 m.b.s., N7=80 m.b.s.

In order to illustrate the movement of water through the profile during the cropping period, figure 6a and 7 contain graphs of water content, θ, and water flux at observation points located at different depths. Both of these graphs reveal that a wetted front advances downwards through the profile, reaching 20 m depth at 8600 hours, 40 m depth at 9200 hours and 60 m at 9700 hours. However, within the three-month fertilizing period the front never reaches the groundwater level, located at 80 m depth.

To illustrate the effect of root uptake on water flow, figure 6b visualizes the same movement of the wetted front as in figure 6a, but with root uptake disabled.



(a) Root uptake enabled. (b) Root uptake disabled

Figure 6. Water content during the cropping period (starting after 7769 hours) for observation nodes at four different depths: N2=20 m.b.s., N5=40 m.b.s., N6= 60 m.b.s., N7=80 m.b.s..

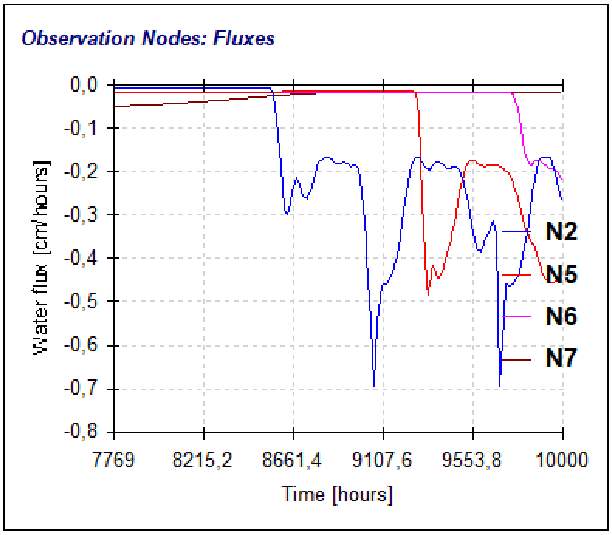
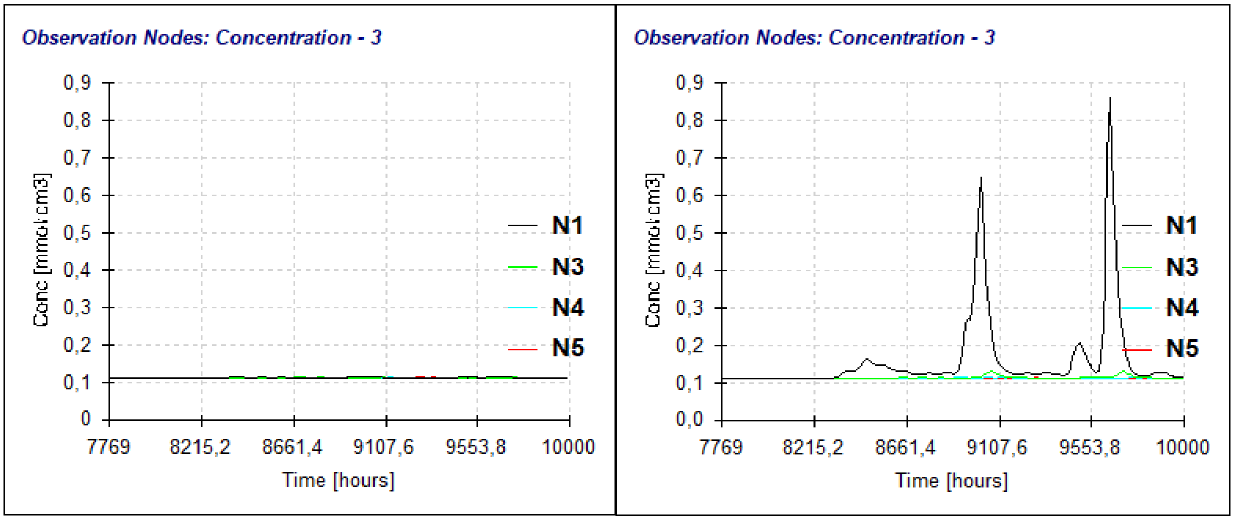


Figure 7. Water flux during the cropping period for observation nodes at four different depths: N2=20 m.b.s., N5=40 m.b.s., N6= 60 m.b.s., N7=80 m.b.s..

4.2. Solute transport

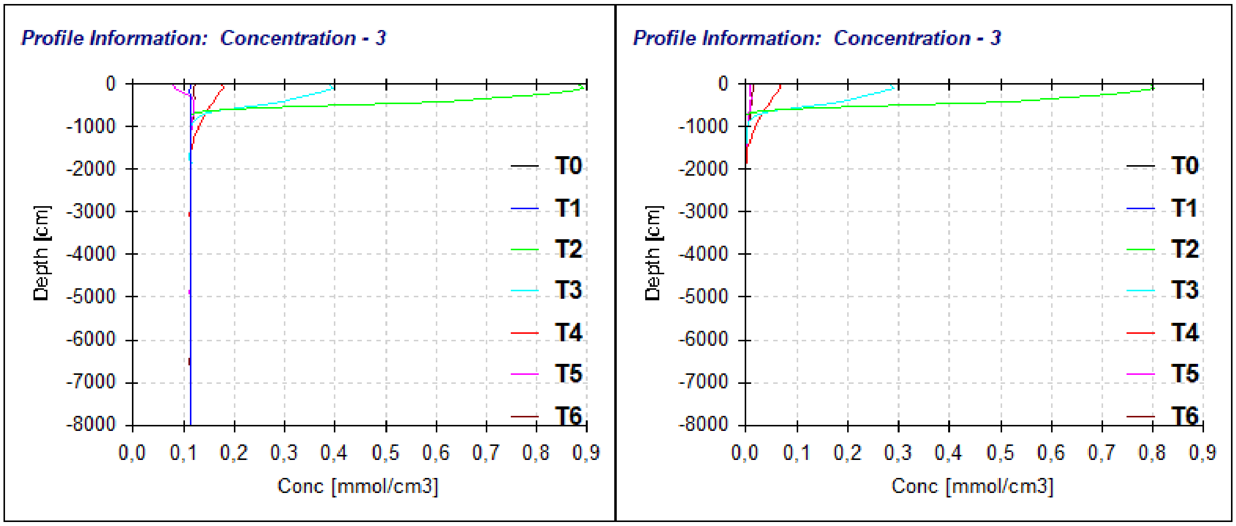
In total, approximately 2100 mmol urea/cm^2 was infiltrated through the soil surface over the three-month cropping period (see fig. 13 in Appendix A2). Breakthrough curves (fig. 8a and 8b) for the different observation nodes give an idea of the infiltration time for nitrate. Both figure 10a and 10b are breakthrough curves for the same points and times, with the difference being the upper boundary condition set for the solute transport. Figure 10a represents the case when a low concentration flux (5 mmol/cm^3) was used for the infiltration of urea, while figure 10b represents the case with high concentration (1000 mmol/cm^3). These graphs have very different characteristics, with the high-concentration case exhibiting significantly larger fluctuations. However, both of them have a horizontal line representing a minimum concentration that seem to be present through the whole simulation period.



(a) Low-concentration case. (b) High-concentration case.

Figure 8. Two versions of nitrate concentrations over the cropping period at four observation nodes at different depths: N1=16 m.b.s., N3=24 m.bs., N4=32 m.b.s., N5=40 m.b.s.. Mineralization is enabled.

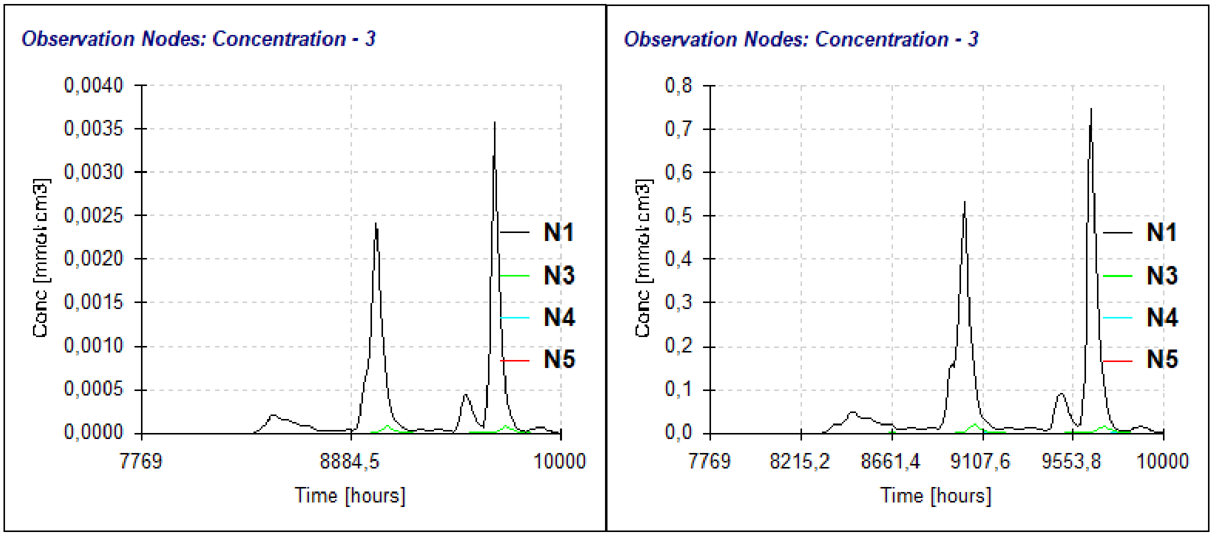
The concentration profiles of nitrate in figure 9a and 9b are included to illustrate the effect that causes this minimum level of concentration. In figure 9a where mineralization is included, it can again be seen as a straight (now vertical) line representing a minimum concentration over the profile at all print times. In figure 9b, where mineralization was disabled, the graphs had the same characteristics but with a shift to the left, so that the minimum concentration was zero.



(a) Mineralization enabled. (b) Mineralization disabled.

Figure 9. Two versions of concentration profiles of nitrate at seven different print times: T0=0 hrs, T1=7760 hrs, T2=8000 hrs, T3=8500 hrs, T4=9000 hrs, T5=9500 hrs, T6=10 000 hrs. Low-concentration case.

Figures 10a and 10b have similar breakthrough curves as in figures 8a and 8b, but when mineralization is disabled. From these it is clear that the breakthrough curves exhibit similar characteristics in both the low- and high-concentration case but with significantly higher nitrate concentrations in the high-concentration case.



(a) Low-concentration case. (b) High-concentration case.

Figure 10. Nitrate concentrations over the cropping period at four observation nodes at different depths: N1=16 m.b.s., N3=24 m.b.s., N4=32 m.b.s., N5=40 m.b.s.. Mineralization is disabled.

The solute concentration profile in figure 11 aims illustrate the effect on nitrate transport from root nutrient uptake. It is the same kind of graph is in figure 9, with the difference being that root uptake is disabled in figure 11.

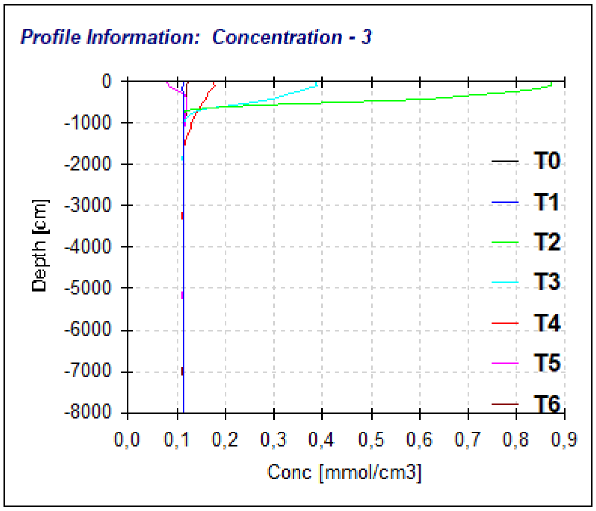


Figure 11. Concentration profile of nitrate at seven different print times: T0=0 hrs, T1=7760 hrs, T2=8000 hrs, T3=8500 hrs, T4=9000 hrs, T5=9500 hrs, T6=10 000 hrs. Root uptake is disabled and mineralization enabled.

5. Discussion

5.1. Interpretation of results

The minimum concentration line that was present in all simulations with mineralization is a source of disturbance in the results. When this is included, a steady flux of nitrate (and ammonium) is present at all times of the simulation (even before urea is applied). The reason to why the mineralization leads to this minimum concentration can be found in the implementation of mineralization in the model. In equation 6, describing the solute transport of ammonium, mineralization is represented by the zero-order rate constant γ_s. Since it is zero-order it is independent of concentration and in Hydrus-1D it is implemented as the term “SinkWater0” for ammonium, which in this model was set to have one value across the whole profile. This means that, regardless of any input of urea, ammonium will at all times be produced from org-N at a constant rate. But instead of accumulating, the coupled reactions of nitrification and denitrification means that an equilibrium concentration is reached in the pore water, as long as no other inputs/outputs of the solute take place. The plausibility of having the same level of mineralization through the whole 80-meter profile should be questioned. It is likely that the organic content of the soil decreases with depth, and that therefore the mineralization rate decreases to negligible levels at larger depths. Also, from the difference in fluctuations between the low- and high-concentration cases, it is clear that the impact of this process on nitrate concentration is dependent on what other sources exist. One such important source is the concentration flux of urea at the top boundary.

A major finding in the simulation results was that neither the water nor the nitrate (apart from that derived from mineralization) reached the groundwater level during the simulation period. An obvious explanation to this is the long extent of the unsaturated zone, which could be seen as a thick protection against groundwater contamination. If the simulation period would have been extended to capture the arrival of the wetted front it is possible that nitrate would have arrived within it but from figure 12 it seems likely that this would not have been with concentrations significantly higher than the concentrations related to the natural process of mineralization.

Another finding was that the time of the breakthroughs is independent of the input concentration of urea, but that only the concentration of the breakthrough pulse is affected. The implication of this finding should not be exaggerated, such that the input concentration is not important. This concentration probably still determines how much ammonia and nitrate is left in the water after root uptake, which can of course be of relevance when assessing groundwater contamination risks.

The two graphs for the case without root uptake (fig. 9 and 13) only show very small differences in water content and nitrate concentration when root uptake is disabled. This is a result which plausibility should be questioned, especially considering that the root depth was 4 meters in the set up.

In general, though, despite that not all of the results are realistic and are built on major simplifications, the end result of the simulations is the provision of results that are, overall, realistic. Thus, it highlights the potential for this kind of modelling for investigating issues related to groundwater contamination. In order to fulfill more of the potential of the modelling approach, though, there are several limitations that do need to be addressed.

5.2. Limitations

Since one of the sub goals of the study was to acquire an understanding of what data is needed to erect a realistic model, it is important to consider the limitations of the simplifications that were made.

A simplification that became relevant early in the study was the characteristics of the soil. The geological profile of the Tiquipaya well (fig. 2) from Renner and Velasco (2000) constituted the foundation from which all of the soil parameters were set. Considering the simplified nature of this foundation (the only basis was the description of the soil as "Boulders, gravel and sand"), one can immediately conclude that this could be a limitation for the study.

Another limitation is related to the parts of the model that describes root uptake of water and nutrients. In this study, very limited data was available in general, and for root uptake no site-specific data was used at all. Here, Hydrus-1D offered useful databases for typical crops with values used in the different uptake models (e.g. Feddes' parameters). However, apart from the use of these values the implementation of root uptake in the model was associated with simplifications. The crops were assumed to be constant over the whole cropping period, meaning that no growth stages were considered. Instead, the crops went from non-existence to being fully grown as soon as the fertilization started. Also, parameters such as albedo, crop height and Leaf Area Index were assumed to be constant over the cropping period (despite that the possibility of using hourly data exist). These simplifications can obviously affect the model's accuracy, considering that both root water and nutrient uptake will be lower in the early stages of a crop's lifecycle, and that parameters like crop height and albedo will affect the evapotranspiration. However, the fact that the root uptake did not appear to have any significant impact on neither water content nor nitrate concentration is probably something that should be further investigated.

Another limitation is the initial conditions of the model, which in this study were set using a pre-simulation. The purpose of the pre-simulation was to compensate for the lack of real data over water content and let a longer period of "natural conditions" set conditions that were representative of reality. However, these "natural conditions" also included several simplifications. Apart from the general inaccuracies related to the modelling approach in general, the pre-simulation period was set up only to include natural precipitation, consequently assuming that no irrigation took place. The water contents that come out of such a pre-simulation could be realistic but will never be as accurate as real data. Additionally, fertilization was not included in this period, and when the cropping period started the concentration of all three solutes was set to be zero. Thus, both for water contents and for solute concentrations, the initial conditions are likely a source of inaccuracy.

For the solute transport part of the model, there were several assumptions which plausibility could be questioned. For instance, the sorption of ammonium was assumed to be linear, meaning that there is no upper limit on how much ammonium could be adsorbed. Also, the simplest model was used for the solute transport - the equilibrium model. This assumes that all adsorption is instantaneous, implying that neither chemical non-equilibrium (involving time-dependent sorption) nor physical non-equilibrium (involving immobile flow regions) exists.

Other simplifications that could be limiting the accuracy are the neglection of hysteresis, the choice of boundary conditions, the values chosen for reaction parameters and timing of the cropping period. The reason to why the timing of the cropping period could be of importance is because different periods are associated with different atmospheric conditions (e.g. dry and rainy seasons).

6. Conclusions

Collection of hydrogeological and hydrogeochemical information (sub goal I) was completed in the first part of the study. However, this part was characterized by a general lack of data, meaning that several aspects of the information had to be predicted with the help of built in modules and databases in Hydrus-1D.

A hypothetical model of how nitrate might interfere with groundwater from the use of fertilizers and flood irrigation (sub goal II) was set up, which included percolation of irrigation water and transformation through the nitrogen chain. This was incorporated into the general conceptual model that was erected in the study (see section 3.2.).

As sub goal IV stated, this conceptual model was then successfully adjusted and combined with relevant (but simplified) data to be set up in Hydrus-1D.

An understanding of the data requirements from Hydrus-1D was acquired, which was what sub goal III set up to do. It was clear that the provision of built-in modules and databases can compensate for a lack of real data, but it was still concluded that it would be preferable to incorporate more real and specific data on for instance soil hydraulic parameters, initial conditions and root uptake.

Regarding sub goal V - about assessing the plausibility of the results - the results were considered plausible in general, but with some flaws that need to be addressed, such as the implication on solute fluxes from a constant rate of mineralization.

In general, then, the study’s purpose was set up to “investigate if one-dimensional modelling of water in the unsaturated zone of the subsoil is useful to assess the transport of contaminants from soil surface to aquifers”. The main conclusion of the study is that the modelling approach has been deemed to possess great potential for that cause, as long as the limitations are addressed in other studies.

6.1. Future studies

In order to improve the accuracy of the model, future studies could try to combine the computer model with field investigations. These could aim to improve the data situation for the input values such as initial conditions, soil hydraulic parameters etc. but could also be used to investigate how well the modelling results correspond to reality. Another idea could be to combine field investigations with the inverse modelling-application of Hydrus-1D in order to calibrate different input parameters. The soil parameters (θ_r, θ_s, $alpha$, n, K_s, $bulk\ density$, $dispersivity$) especially, would benefit from further research. At the moment they have been derived in a very simplified manner (see section 5.2) despite being important parameters that could be determined quite straightforwardly with field investigations.

Also, the part of the model that deals with root uptake might need further work. The findings of this study that root uptake does not influence water contents or nitrate concentrations significantly is not very realistic.

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Appendix

A1 List of all settings used in the Hydrus-1D model

Main Processes

Simulate: **Water flow**, **Solute transport** and **Root water uptake**

Geometry Information

Number of soil materials: 1
Number of layers of mass balances: 1
Decline from vertical axis: 1 (vertical)
Depth of soil profile: 8000 cm

Time Information

Time unit: minutes
Initial time: 0
Final time: 10 000 hours
Initial time step: default
Min. time step: default
Max. time step: default
Time variable conditions: 10 000
Meteorological records: 10 000
⇒ **Penman-Monteith equation**

Print Information

Default

Water Flow - Iteration Criteria

Default

Water Flow - Soil Hydraulic Property Model

Single Porosity Model **- van Genuchten-Mualem**
No hysteresis

Water Flow - Soil Hydraulic Parameters

Material 1 - Layer of boulders, gravel and sand

Using Rosetta module (neural network prediction) sand/silt/clay: 90/5/5 %
⇒

Mat	Qr [-]	Qs [-]	Alpha [1/cm]	n [-]	Ks [cm/min]	I [-]
1	0,0515	0,3769	0,0332	2,5032	0,223618	0,5 (default)

Water Flow - Boundary Conditions

Upper: **Atmospheric with surface layer**
Lower: **Constant pressure head**
Initial condition: **in pressure heads**
Max h at surface: **20 (cm)**

Solute Transport - General Information

Time weighting scheme: Crank-Nicholson
Space weighting scheme: Galerkin finite elements
Mass units: mmol
Stability criterion: 2
Dependence of env. Factors: **none**
Solute transport model: **equilibrium model**
Iteration criteria: default
Tortuosity: ⇒ **use tortuosity factor, Millington-Quirk**
Number of solutes: **3**
Pulse duration: **0**

Solute Transport - Transport Parameters

Soil specific parameters

Hydrus variable	**Value**	**Source**
Bulk.D	1,5*10^{-6} g/ cm^3	**(Gonzales Amaya, Barmen and Muños, 2018)** “1.3-2.0 g/cm3 Range of densities for gravel-sand levels of at least 60 weigth%”
Disp.	800	**(Beven 1993, Cote 2001, Cote 2003)** 1/10th of prof.length
Frac = 1	1	-
Thlm = 0	0	-

Solute specific parameters

Sol.	**Diffus. W. [cm2/d]**	**Diffus. G.**	**Source**
1	1,194048	non-volatile	(Winkelmann, 2017)
2	1,52	18057,6	(Li et al., 2015)
3	1,64	non-volatile	(Li et al., 2015)

Solute Transport - Reaction Parameters

Urea (1)

All zero except:

Variable	Hydrus variable	Value	Source
$\mu'_{w,1}$	SinkWater1’	0.38 day^{-1}	(Hanson et al. 2006)
	Alpha	0	

Ammonia (2)

All zero except:

Variable	Hydrus variable	Value	Source
$K_{d,2}$	Kd	3.5 cm^3/g	(Ling and El-Kadi, 1998)
	Nu	0	
	Beta	1	
	Henry	0.000295 (at 25°C)	(Li et al., 2004)
$\mu'_{w,1}$	SinkWater1’	0.2 day^{-1}	(Hanson et al. 2006)
$\gamma_{w,2}$	SinkWater0	0.0045 day^{-1} (0 when mineralization disabled)	(Li et al., 2015)
	Alpha	0	

Nitrate (3)

All zero except:

Variable	Hydrus variable	Value	Source
$\mu_{w,3}$	SinkWater1	0.04 day^{-1}	(Li et al., 2015)
	Alpha	0	

Solute Transport - Boundary Conditions

Upper: **stagnant BC for volatile solutes**

Lower: **Zero concentration gradient**

Stagnant boundary layer: **0.02**

Conc. in atmo: 0

Initial: In liquid phase conc.

Root Water Uptake - Models

Water Uptake Reduction Model: **Feddes**

Solute Stress Model: **Multiplicative Model ⇒ Threshold Model**

Critical Stress Index for Water Uptake: **1**

Root Solute Uptake Model: ⇒ no Active Solute Uptake

Maximum Allows Conc. for Passive Uptake:

Sol. No.	**cRoot**
1	0
2	1000
3	1000

Root Water Uptake - Water Stress Reduction

Feddes Parameters:

P0 [cm]	-15	No uptake above this pressure head (h)
P0 pt [cm]	-30	Maximum uptake below this h
P2H [cm]	-550	Maximum uptake above this h (for r2h)
P2L [cm]	-650	Maximum uptake above this h (for r2L)
P3 [cm]	-8000	No uptake below this h (wilting point)
r2H [cm/min]	0.5	
r2L [cm/min]	0.1	

Source: Database in GUI for “Onions - bulbing time”

Root Water Uptake Parameters

Threshold = 2.4

Slope = 8

Osm. coeff. = 1 (for all three solutes)

Source: Database (in GUI) for “Onion”

Variable Boundary Conditions

Time [hours]: 1-10 000

Precip. [cm/hour]: *from meteorological data (Asaana meteorological station)*

hCritA [cm]: -50 000 *for all data points*

cTop-1: 0 *for all data points where irrigation=0,* 5 *or* 1000 *for data points with irrigation*

cBot-1/cTop-2/cBot-2/cTop-3/cBot-3: 0 *for all data points*

Meteorological Parameters

Radiation

⇒ Solar radiation

Geographical and Meteorological Parameters

-17.4223 Latitude (deg, N+, S-)
2570 Altitude [m]
0.25 Angstrom value a
0.5 Angstrom value b
0.9 a1
0.1 b1
1.35 ac
-0.35 bc
0.34 al
-0.139 bl
200 Wind speed (measurement height) [cm]
200 Temperature (measurement height) [cm]

Cloudiness

⇒ Solar radiation
⇒ Relative humidity

Crop data ((dry)onion)

⇒ **Tables** (growth data, below)

Growth data:

	Time [hour]	Crop height [cm]	Albedo [-]	LAI/SCF [-]	Root depth [cm]
1	0	0	0,23	0	0
2	7768	0	0,23	0	0
3	7769	40	0,23	136,9	40
4	10000	40	0,23	136,9	40

Meteorological Conditions

From meteorological data (Asaana meteorological station)

Soil Profile

Initial conditions

Water content: 0.1 *across whole profile*
Root distribution: 1 *at 0-400cm depth*

A2 Graphs of cumulative fluxes

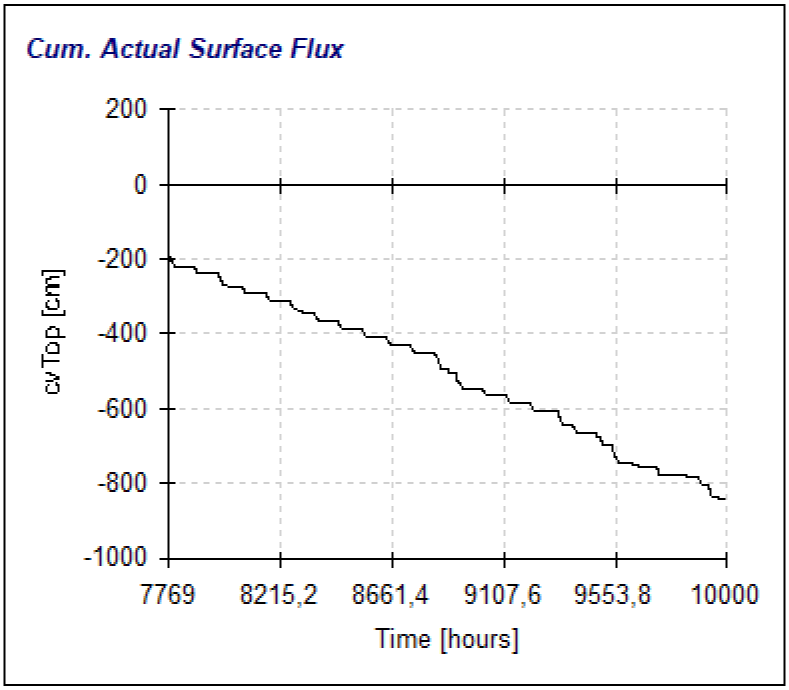

Figure 12. Cumulative actual surface water flux over the three-month cropping period. The difference in "cv Top" between time=10000 hours and time=7769 hours represents the infiltrated volume per area unit.

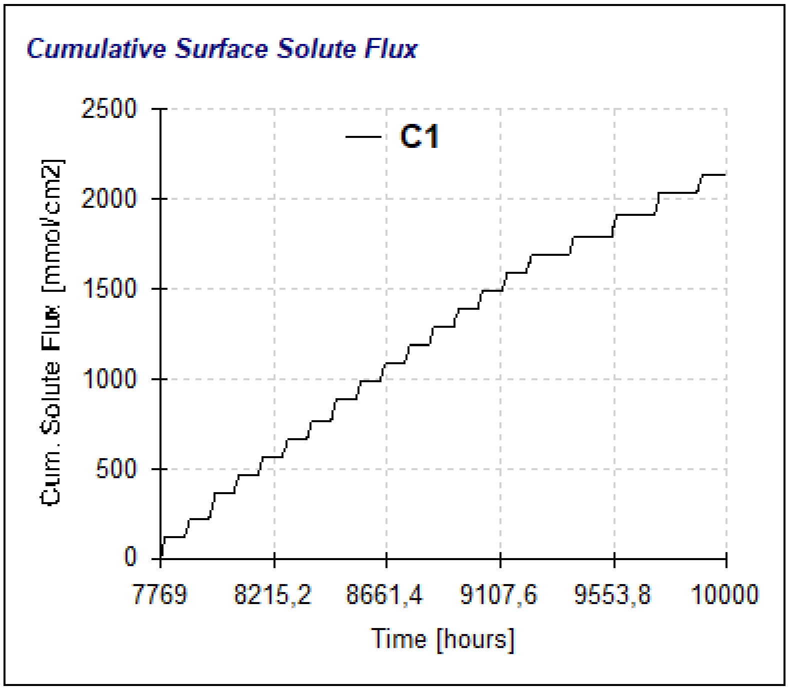

Figure 13. Cumulative surface solute flux (of urea) over the three-month cropping period. It represents the molar amount infiltrated per area unit.