Numerical Modeling of Water Flow and Contaminant (Nitrates) Transport in Agriculture: Review

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Summary

Water movement in soils is a key process that affects water quantity and quality in the environment. Movement of contaminants in soils is closely linked with the soil water flux and it is very important to properly evaluate these processes that occur in vadose zone. With development of new technologies more attention is dedicated to the use of numerical models to assess water flow behavior and groundwater pollution caused by agricultural production. This paper presents a review of many articles that are focused on vadose zone modeling and on the application of these models in agricultural/environmental sciences. With increasing development of computer technologies there is also increasing amount of programs that solve water flow and solute transport. Water flow is solved with Richard's equation, and for space discretization Galerkin finite element method is mostly used. The equation used in solute transport dominantly depends on solute whose transport is simulated. Modeling for sure represents the future of environmental protection and can be used for better understanding of vadose zone processes.

Key words

vadose zone, numerical modeling, agriculture

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Introduction

During the past decades many models with varying complexity and dimensionality have been developed to quantify the basic physical and chemical processes that can affect water flow and solute transport in the vadose zone. These models are now increasingly used in science, research, and management of ecosystems. With development of computers there was also increased use of numerical models that can solve complex mathematical equations quickly and efficiently. Numerical models are becoming much more complex and can now be applied to one-, two-, and three- dimensional problems of (un)saturated water flow, heat flow, and solute transport. These models describe processes in soils based on well-known laws and equations. Some of the modeling tools can be quantitative-empirical. Nowadays there are many commercial and public domain numerical models (programs) that can be used for a prediction of soil properties and processes in soils and groundwater. Selection of the proper model for a specific problem should be based on: spatial and time scale, available data set, possibility of a new data addition, required quality and precision of resulting information etc. (Kozak et al., 2010). Models that were mostly used until now are called single-porosity models. Newly developed models are based on concepts of dual-porosity, dual-permeability, multiple-porosity, and multiple-permeability. The basic assumption is that each domain is characterized by its own set of transport properties and equations that describe water flow and transport processes. This paper focuses on: (i) main equations that are used for modeling water flow and solute transport, (ii) state of the art numerical programs used for solving processes in vadose zone, and (iii) review of simulation of nitrogen dynamic in agricultural soils.

General equation used in numerical models

Water flow is one of the most important processes in vadose zone and it is described with Richard's equation:

$$\frac{\partial\theta(h)}{\partial t} = \frac{\partial}{\partial z}\left(K(h)\frac{\partial h}{\partial z} + \frac{\partial K(h)}{\partial z}\right) - S(h) \qquad (1)$$

where θ is volumetric water content [L^3L^{-3}], t is time [T], z is vertical coordinate positive upwards [L], h is pressure head [L], and S is sink term (root water uptake) [T^{-1}]. The Richard's equation is based on the continuity equation and Darcy's law, which expresses a water flux density as a function of a potential gradient:

$$\frac{\partial\theta}{\partial t} = -\frac{\partial q_z}{\partial z} \qquad (2)$$

$$q_z = -K\frac{\partial H}{\partial z} \qquad (3)$$

where H is sum of pressure (h) and gravitational (z) head [L], and q_z represents flux densities [LT^{-1}]. Two soil hydraulic properties must be known to solve this equation and to simulate water flow in soils. They are soil-water content retention curve and a hydraulic conductivity curve. The Richard's equation expression for the three-dimensional system can be simplified assuming following factors: (i) water flow is either steady or unsteady in time, (ii) soil porosity is either homogeneous or heterogeneous, (iii) soil porosity system is isotropic or anisotropic, (iiii) water flow is in one- two- or three- directions.

Transport of various substances are associates with the water flow. Some of them dissolve in water and then they are transported in soils. On the other hand some of substances are not dissolved in water and they are simultaneously transported with water through soil profile. Substances either do not react with soil and do not change in time, or react with soil particles and change due to chemical reactions, microbiological transformation etc. According to the substances type the solute transport is either conservative (substances do not vary in time due to different reactions) or non-conservative (substances content varies; adsorption, degradation, volatization, denitrification, nitrification, chemical dissolution etc.).

Main equation for describing solute flux:

Advection:

$$q_a = q_c \qquad (4)$$

Hydrodynamic dispersion:

$$q_d = -D\theta\frac{\partial c}{\partial z} \qquad (5)$$

Continuity equation:

$$\frac{\partial(\theta c)}{\partial t} = -\frac{\partial(q_d+q_a)}{\partial z} \qquad (6)$$

where q_a is solute flux density due to advection [$ML^{-2}T^{-1}$], q_d is solute flux density – hydrodynamic dispersion [$ML^{-2}T^{-1}$], c is solute concentration [ML^{-3}], q is water flux density [LT^{-1}], D is dispersion coefficient [$L^{-2}T^{-1}$], θ is soil water content [L^3L^{-3}], z is the coordinate [L].

Advection-dispersion equation:

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial(\rho s)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D\frac{\partial c}{\partial z} - qc\right) - \emptyset \qquad (7)$$

where c is solution concentration [ML^{-3}], s is adsorbed concentration [MM^{-1}], Ø is water content [L^3L^{-3}], ρ is soil bulk density [ML^{-3}], D is dispersion coefficient [$L^{-2}T^{-1}$], q is volumetric flux [LT^{-1}], and θ is rate constant representing reactions [$ML^{-3}T^{-1}$].

Modeling of water flow and transport of contaminants

Simulation of water flow and transport of contaminants have an increasingly important role in the modern approach for protection of water resources and sustainable agricultural production (Barry, 1992; Šimůnek and Bradford, 2008). Because of the importance of unsaturated zone as an important factor of maintaining ecosystems on Earth (Brussaard et al., 2007) there is a great need for understanding and predicting the complex interactions in vadose zone including the biochemical reactions (Wissmeier et al., 2009). In recent years there has been increasing attention to vadose zone, where the contamination can still be diminished before it reaches the groundwater. Development of new computer technology have been increasing in past few years and many programs that can numerically solve the problems of movement of water, heat, and pollutants in the (un)saturated zone. Šimůnek and Bradford (2008) presented an overview and examples of the development of a large number of well-known

Table 1. Examples of used programs and models for simulations of the movement of water and transport of contaminants

Software name	Used numerical model	Author	Dimensions (1D/2D/3D)	Soil structure	Inverse method	Soulte concentration (Freundlich, Langmuir and linear)	First order rate reactions	Transpiration	Nutrient uptake	Applicability
PASTIS Predicting Agricultural Solute Transport in Soils	Finite element method	Lafolie, 1991	1	x	–	–	x	x	x	Water flow, Ca, Mg, Na, K, Cl, SO_4, Si
SWAP Soil Water Atmosphere Plant	Finite element method	van Dam i sur., 1997	1	x	–	x	x	x	x	Water flow, transport of heat and inorganic compounds
HYDROGEOCHEM hydrologic transport and geochemical reaction model	Finite element method with rectangular and triangular discretization	Yeh and Salvage, 1996	3	x	x	–	–	–	–	Water flow, transport of heat, organic and inorganic compounds
LEACHM Leaching estimation and chemistry Model	Finite element method	Hutson and Wagener, 1992	1	x	x	x	x	x	x	Water flow, nitrogen and pesticide dynamics, microbiological reactions, inorganic compounds
MACRO	Finite element method	Jarvis, 1991	1	x	–	–	–	x	x	Water flow, evapotranspiration, transport of organic and inorganic compounds
HYDRUS-1D HP1- PHREEQC	Galerkin's finite element method	Jacques i Šimůnek, 2005 (Parkhurst and Apello, 1999)	1	x	x	x	x	x	x	Water flow, transport of heat and inorganic compounds, evapotranspiration, with PHREEQC solving geochemical and microbiological reactions
HYDRUS-2D		Šimůnek et al., 1999	2	x	x	x	x	x	x	
HYDRUS-3D		Šimůnek et al., 2006	3	x	x	x	x	x	x	
FEFLOW Finite Element subsurface FLOW system	Finite element method	Dierch, 2002	3	x	x	x	x	x	x	Water flow, transport of heat and inorganic compounds

computer tools that are used to study water flow and transport of contaminants in vadose zone, which can be used in agriculture. These tools include numerical models for one-or multi-dimensional (un)saturated water flow and transport of contaminants in the software packages (HYDRUS-1D, HYDRUS-2D, HYDRUS-3D, Šimůnek et al., 1999, 2006); analytical models for the transport of contaminants in soil and the groundwater (CXTFIT, Toride et al., 1995; STANMOD, Šimůnek et al., 1999) and codes and tools and databases for analysis and prediction of soil hydraulic properties (RETC, Van Genutchen et al., 1991; ROSETTA, Schaap et al., 2001, and UNSODA, Leij et al., 1999). These models cover a large number of possibilities for solving transport problems, from relatively simple problems like one-dimensional transport of contaminants to solving complex problems of multidimensional flow and transport of contaminants, including a large number of complex biogeochemical reactions. An example is the HP1 model that can solve transportation of major chemical compounds (Jacques et al., 2008), which can be used as part of a software package HYDRUS using PHREEQC tools for modeling of geochemical processes (Parkhurst and Appelo, 1999).

Finsterle et al. (2008) in their paper presented TOUGH program that solves the problems of water flow and transport of contaminants. TOUGH program includes several modules that solve problems nonizotermal multiphase flow (TOUGH2, T2VOC), reactive biogeochemical transport (TOUGHREACT), and mechanical processes in rocky materials (TOUGH-FLAC). Panday and Huyakorn (2008) describe the program MODFLOW SURFACT, which includes modules that have been developed for the software package MODFLOW (Harbaugh et al., 2000) that is used for modeling of groundwater flow. Program MODFLOW SURFACT is used for simulation of unsaturated flow, degree of infiltration of precipitation, and/or leaching and transport of contaminants. For simulating groundwater flow in water well in Međimurje County (Croatia) Posavec and Mustač (2009) successfully used MODFLOW software package. Healy (2008) gives a brief overview of the approach for simulation movement of water, solute, and heat through (un)saturated media, including a brief description of the most commonly used models for this purpose. Further examples include program VS2DTI (Hsieh et al., 1990) that is used for two-dimensional flow modeling and transport of contaminants in the soil profile in two-dimensional plane. The program is used to simulate the unsteady water flow and transport of contaminants in variably (un)saturated porous media. Van Dam et al. (2008) present an overview of the main and auxiliary one-dimensional features of the SWAP model. Processes of water movement, heat, and transport of contaminants in (un)saturated zone are solved similarly to the above described models. Additional special functions that are involved in the SWAP program include the growth of crops, the processes of gathering, and dissemination of soil aggregates and water movement through macropores and the interactions between surface water and groundwater. Voss et al. (2002) described the program SUTRA

(Saturated-Unsaturated Transport) that is used for simulation of the movement of fluids and transport of energy or dissolved substances in the underground. Groenendijk et al. (2005) described in their research program ANIMO, which is used to evaluate the leaching of nitrates /phosphorus and monitoring of their loads in surface and groundwater. This program is used primarily to evaluate the use of fertilizer on a regional and national level. ANIMO enables quantification of the leaching of nutrients from agricultural land and greenhouse gas emissions that occur as a result of the high amounts of applied fertilizer and inadequate protection of soil and water. The program is used to quantify the components of the carbon cycle, the nitrogen, and phosphorus in the saturated and unsaturated conditions. Another program that is used often in agriculture is MACRO (Jarvis et al., 1991), which is used to simulate one-dimensional water flow and reactive transport in different soil types. MACRO describes the flow of water through the soil structure that is divided into two zones (macropores and micropores), and for each zone model calculates velocity of flow and transport of substances. Additional capabilities in simulations are evaluating the process of degradation of pesticides based on first-order kinetic reactions including sorption simulation based on Freundlich and Langmuir isotherm in both porous systems. The program is mostly used in agriculture to simulate the behavior of pesticides in different soil types (Armstrong et al., 2000; Gottesbüren et al., 2000; Thorsen et al., 1998; Villholth et al., 2000) and in research of impact by irrigation on leaching of contaminants in the soil zone (Andreu et al., 1996; Bourgault de Coudray et al., 1997).

Software package LEACHM (Hutson et al., 1992) is based on four simulation modules that are used to simulate vertical movement of water and substances. These modules differ in the description of the process of chemical equilibrium, transformation and degradation of the substances. LEACHW is used for water flow simulations. Other models describe pesticide degradation (LEACHP), nitrogen and phosphorus (LEACHN) and the degree of salinity in calcareous soils (LEACHC). Jabro et al. (1995) in their research evaluated the module that is based on Richard's equations and advection and dispersion equation (LEACHN). Estimated LEACHN module is used to simulate nitrate leaching based on field data from five field trials. It was found that the model is unreliable for the simulation of nitrogen transformations in soils. Table 1 presents some of the most widely used software packages in the field of agriculture, which are based on Richard's equations and advection/dispersion equations.

Modeling nitrogen dynamics with HYDRUS

Some of the most advanced and most widely used software packages are HYDRUS-1D and HYDRUS 2D/3D (Šimůnek et al., 1999), which are based on the application of Galerkin-type linear finite element method. HYDRUS-1D program is used for modeling.water flow and transport solutions in the (un)saturated media in one-dimensional plane. HYDRUS-2D/3D enables the use of models in two-dimensional (axsymmetrical) and three-dimensional plane (Šimůnek et al., 2006). The numerical model allows specification of plant root distribution and water and nutrients plant uptake in relation to the distribution of irrigation or rainfall. Model is successfully used to simulate the application of fertigation and transport processes of nitrogen species that are indicated in many papers (Ajdary et al., 2007; Crevoisier et al., 2008; Hanson et al., 2006; Mailhol et al., 2001). Also, the programs have been used for simulations using data from field lysimeters in describing the process of movement of water and contaminants using stable isotopes (Stumpp et al., 2012). Luo and Sophocleous (2011) conducted a calibration of model using data from the zero tension lysimeters, after which they conducted various simulation of calculation of evaporation at different depths and different amounts of water (rain and irrigation). Gärdenäs et al. (2005) examined the impact of low volume irrigation and soil type on nitrate leaching potential for four different irrigation systems, also with the help of the program HYDRUS-2D.

Ravikumar et al. (2011) estimated transformation and transport of urea in the area of sugar cane in the system of drip irrigation and quantifed the flows of urea, ammonium nitrate, and ammonium volatilization using numerical simulations. Typical scenarios, which are based on recommended dosage of urea for use in the system of drip irrigation, are tested using the program HYDRUS-2D. The total amount of fertilizer applied was divided into 49 doses, depending on the stage of plant development. Simulations were including in the application of irrigation and fertilization. Irrigation schedule that allows the application of 30% less urea was developed, and thereby provides a sufficient amount of nutrients in all the developmental stages of the plant growth. Hanson et al. (2006) conducted a study in which with the application of program HYDRUS-2D they tried to simulate the application of micro fertigation with increased productivity and elimination of negative environmental factors. They estimated that the numerical model is an efficient tool to evaluate the strategies of irrigation and fertilization with urea. The model successfully described transport of urea, ammonium and nitrate in irrigation taking into account the processes of hydrolysis and nitrification of ammonia adsorption on soil particles. Hanson et al. (2004) examined the impact of the application of fertigation and soil type on nutrient availability and leaching using computer simulations, which are used to estimate the distribution of nutrients in the nearest surrounding of drippers used for irrigation.

In the first phase of the simulations they have researched distribution of nitrate in five different watering schedules with four different types of low volume irrigation on four types of soil. The second phase included distribution of fertilizer phosphorus, potassium, ammonia, and urea in three differently scheduled applications, two types of low volume irrigation and in one soil type. In conclusion the authors stated that the application of fertilizer at the beginning of the irrigation cycle increases leaching and that the annual leaching is greater in soils that have a coarser (sandy) texture. Ammonia, phosphorus and potassium are strongly adsorbed to soil particles so that the irrigation schedule had very little effect on their distribution in the soil profile. Bolado Rodríguez et al. (2010) conducted a study in which they applied two types of slurry in the soil column in laboratory. With using HYDRUS-1D program they simulated degradation process of slurry and ammonia adsorption. In their research, Ramos et al. (2011) simulated the movement of contaminants in field conditions in Portugal. The authors conducted a complex experiment involving the application of saline irrigation water with different doses of nitrogen.

The model successfully simulated the adoption of water and nutrients through the roots. HYDRUS-1D program proved to be a reliable tool for assessing the concentration of substances associated with soil salinity and nitrogen compounds. Wang et al. (2010) conducted a study in which they tried to assess the possibility of leaching of nitrogen accumulated in the soil profile and the usefulness of the application of Br^- as tracer with surface application of nitrogen-based fertilizers during major rainfall or irrigation. They conducted an experiment in three variants with respect to the amount of water: a) only precipitation, b) +100 mm rainfall irrigation, and c) +500 mm rainfall irrigation. Movement of $Br^-$and NO_3^-, which were applied to the surface were simulated with HYDRUS-1D. Simulations have shown that Br^-quickly moved through the soil profile of NO_3^- ions. It was found that the greater the initial content of nitrogen in the soil, leaching was higher, also much greater leaching was associated with increased rainfall and water due to irrigation. Köhne et al. (2005) examined the long-term movement of soil nitrate and nitrate metabolism. HYDRUS-2D program was applied, which is augmented with a relatively simple model (MIM), which simulates the metabolism of nitrogen in soil and free water in the soil. This model, based on observations of ten years on leaching from drainage systems, simulated aerobic and anaerobic conditions that control the metabolism of nitrogen. The results showed that the content of nitrogen and nitrates concentrations was significantly increased in the period and in the part of the profile that had a larger amount of free water.

Conclusions

It is obvious that the transport processes (water flow and solute transport) in vadose zone is a very complicated and complex problem. Before the transport equations could only be solved analytically, now with a development of computer technologies there is possibility to solve complex problems numerically in short time and with greater accuracy. In few recent years there has been also a large number of models (ANIMO, MACRO, LEACH, HYDRUS 1D, etc.) that are freeware programs and they are available to everyone. This fact leads to improvement of new and very complex programs for solving large variety of problems associated with water flow and solute transport in (un) saturated soil conditions. As our knowledge in the vadose zone processes rises there is a possibility to incorporate new knowledge in development of new models that can be used in science but also in achieving greater crop yields and in preserving ecosystems from pollution.

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