REVIEW OF SOFTWARE FOR MODELING MIGRATION OF EMERGING CONTAMINANTS IN GROUNDWATER

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Introduction

The presence of organic pollutants in aquatic environments has been of great concern worldwide for years, especially in connection with the quality of the soil-groundwater environment. Increasing numbers of different types of emerging contaminants (ECs) e.g. pharmaceutical compounds, pesticides or endocrine disrupting compounds, have been identified and investigated in aqueous environments over recent decades. Since groundwater is widely used for drinking water supplies, their contamination can be a major source of human uptake of organic pollutants. Therefore, it is important to have a detailed understanding of the distribution and transport of these compounds in groundwater, in order to guarantee safe drinking water for people in the future. The main pathway of ECs to get into the aquatic environments is through discharge from sewage treatment plants (Banzhaf and Hebig, 2016). Although techniques exist for removing organic micropollutants during wastewater treatment standard wastewater treatment plants do not usually completely remove all of them. Accordingly, this implies that such substances are still continuously released into the aquatic environment and their concentrations are increasing rather than decreasing (Münze et al., 2017). Emerging contaminants can also enter aquatic environments from livestock farming, landfill sites, wastewater irrigation of fields, leaking sewers, and on-site water treatment units and septic systems (Banzhaf and Hebig, 2016).

Samples and methods

Because it is usually not possible to carry out experimental investigations at long enough distances or time periods, the fate of contaminates is tested on a laboratory scale using, for example, column experiments (Zakari et al., 2016). The laboratory tests can be used further as an efficient method to provide input data for numerical modeling of ECs (reactive tracers) transport and fate in the soil-water system. The computer simulation methods require, apart from defining boundary conditions, knowledge of flow and transport parameters (Witczak et al., 2013). Progress in the software now allows simulation of pollutant transport in the aquifer by means of advanced mathematical models. The aim of this paper is to summarise the results of literature research regarding the software for modelling the migration of organic substances in groundwater. For this purpose, a literature review was conducted using the available sources of scientific research (Web of Science, Science Direct, Scopus, Google Scholar).

Results

A large number of computer programs exists for evaluating ECs transport in porous media using different analytical solutions, such as CXTFIT, STANMOD, HYDRUS-1D, which are the most commonly used, as well as PHREEQC, The Geochemist's Workbench, Processing MODFLOW with MT3D module, GMS, and FEFLOW. This programs enable to calculate values of transport parameters, such as the pore-water velocity, the retardation factor, dispersion coefficient, and degradation or production parameters.

The CXTFIT is the computer software frequently used to fit the convection-dispersion equation CDE to observed breakthrough curves (Toride et al, 1995), which is available in various forms, for example through the public domain STANMOD software (Simunek et al., 1999). This model has been widely used to estimate e.g. pesticide transport parameters (Rodríguez-Liébana et al., 2018) during steady one-dimensional flow. The inverse problem is solved by minimizing, using non-linear least squares, an objective function that consists of the sum of the squared differences between observed and fitted concentrations.

The free HYDRUS-1D software is also commonly used for determination of transport parameter e.g of pharmaceuticals (Martínez-Hernández et al., 2017). This software tool numerically solves the Richards equation for variably saturated water flow and advection-dispersion type equations for solute transport (Šimůnek et al., 2005).

Conclusions

Based on literature research, a large number of computer programs exists for evaluating ECs transport in porous media using different analytical solutions. Unfortunately, it is generally difficult to obtain reliable values of transport parameters, such as the pore-water velocity, the retardation factor, dispersion coefficient, and degradation or production parameters. Therefore, there is a necessity to combine laboratory and modeling data to verify the correctness of the received transport parameters.

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