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Challenges in modelling dissolved organic matter dynamics in agricultural soil using DAISY

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Abstract

Because dissolved organic matter (DOM) plays an important role is terrestrial C-, N- and P-balances and transport of these three components to aquatic environments, there is a need to include it in models. This paper presents the concept of the newly developed DOM modules implemented in the DAISY model with focus on the quantification of DOM sorption/desorption and microbial-driven DOM turnover. The kinetics of DOM sorption/desorption is described by the deviation of the actual DOM concentration in solution from the equilibrium concentration, C_{eq}. The C_{eq} is soil specific and estimated from pedotransfer functions taking into account the soil content of organic matter, Al and Fe oxides. The turnover of several organic matter pools including one DOM pool are described by first-order kinetics.

The DOM module was tested at field scale for three soil treatments applied after cultivating grass–clover swards. Suction cups were installed at depths 30, 60 and 90 cm and soil solution was sampled for quantification of dissolved organic C (DOC) and dissolved organic N (DON). In the topsoil, the observed fluctuations in DOC were successfully simulated when the sorption/desorption rate coefficient k was low. In the subsoil, the observed concentrations of DOC were steadier and the best simulations were obtained using a high k. The model shows that DOC and DON concentrations are levelled out in the subsoils due to soil buffering. The steady concentration levels were based on the C_{eq} for each horizon and the kinetic concept for sorption/desorption of DOC appeared a viable approach. If C_{eq} was successfully estimated by the pedotransfer function it was possible to simulate the DOC concentration in the subsoil. In spite of difficulties in describing the DOC dynamics of the topsoil, the DOM module simulates the subsoil concentration level of DOC well, and also—but with more uncertainty—the DON concentration level.
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1. Introduction

Dissolved organic matter (DOM) is an important contributor to transport of nutrients in the soil system (Guggenberger and Kaiser, 2003). Export of DOM and associated N and P from soils to surface waters may contribute substantially to eutrophication (Stepanauskas et al., 2002). Dissolved organic carbon (DOC) concentrations in 22 UK upland waters have increased by an average of 91% during the last 15 years and there is evidence of similar changes at other monitoring sites across Europe and North America. Long-term DOC leaching may have wide-ranging impacts on freshwater biota, drinking water quality, coastal marine ecosystems and upland carbon balances (Evans et al., 2005).

Soil solutions contain varying amounts of DOM, which originates from plant litter, soil humus, microbial biomass,

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and from root exudates (Kalbitz et al., 2000), but the quantitative contribution made by each of these sources is controversial and differs depending on the definition and methods used for determination of DOM (Zsolnay, 1996). Microbial control of DOM production is frequently mentioned in studies of DOM cycling. Hence, Guggenberger et al. (1994) found that the chemical composition of DOM fractions indicated that DOM is mainly comprised of by-products of organic matter mineralization and of products of microbial synthesis. In 14 old agricultural fields that had been abandoned, Zak et al. (1990) observed that water-extractable C and microbial biomass C were highly correlated and the water-extractable C was about 20% of microbial biomass C. On the contrary, Zsolnay (1996) stated that the largest and most consistent source of DOM presumably is the immobile SOM, which is approximately 100-fold more abundant than the DOM itself. Findings of ^{14}C studies by Trumbore et al. (1992) and Tegen and Dorr (1996) suggest that mobile DOM is produced from rather old fractions of organic material.

Evidence from studies in soil systems indicates that sorptive protection of DOM may be of particular importance. According to several authors (e.g. Guggenberger and Zech, 1992; Qualls and Haines, 1992; Kaiser et al., 1996) the change in concentration of DOM during transport through the mineral soil is caused by sorption of DOM on to the mineral phase. Iron and aluminium oxides are important sorbents of DOM with sorption usually described as surface complexation of DOM carboxylic acid groups (Kaiser et al., 1997). Additionally, it is often found that soil is able to release DOM when exposed to aqueous solution containing no or very low concentrations of DOM (Nodvin et al., 1986; Kaiser, 2001; Gjettermann et al., 2007). Thus, the soil solid phase may not only sorb DOM but may also release it.

Modelling has become an important tool in studies of soil nutrients, be it nutrient uptake by crops or losses by leaching to the environment. The issue of identifying and particularly quantifying the sources of DOM in soil is rather challenging and different approaches have been developed. In the ANIMO model, described by Groenendijk and Kroes (1999), manure and slurry contains a soluble organic fraction that is added to the DOM pool when applied. Additionally, decomposition of fresh organic material results in production of DOM. On the other hand, microbial production of DOM is the only source of DOM in the CENTURY model (Parton et al., 1994). The DyDOC model (Michalzik et al., 2003, Tipping et al., 2005) and the model described by Neff and Asner (2001) also include physical/chemical sorption of DOM in soil. In the DyDOC model, the DOM sorption is described by an equilibrium partitioning coefficient where the parameterization of the partitioning coefficient accounts for differences in soil pH, Al concentration in soil solution, DOC properties and the nature of soil solids (Lofts et al., 2001a, b). In the model described by Neff and Asner (2001) it is assumed that DOM sorption at equilibrium is described by the initial mass-isotherm. If water flow occurs, the isotherm is modified and kinetic considerations are included, by use of a very simple algorithm.

Process descriptions for DOM dynamics were recently included in the DAISY model. The DAISY code (Hansen et al., 1990, 1991; Abrahamsen and Hansen, 2000) has been validated at several occasions (e.g. Shaffer et al., 2001) and has always been evaluated favourable, in particular with regard to simulation of nitrogen and carbon transformations in soil (de Willigen, 1991; Vereecken et al., 1991; Diekkrüger et al., 1995; Smith et al., 1997). This paper presents the concept of the newly developed DOM module in the DAISY model, which was tested with field data from a study on DOM mobilization and transport after cultivating grass–clover swards (Vinther et al., 2006). In this model DOM is defined as dissolved organic substances passing through a 0.45 μm filter. In the present paper, the effect of soil treatments on the simulated DOM dynamics is investigated with special focus on the importance of DOM sorption/desorption in relation to microbial-driven DOM turnover.

2. Materials and methods

2.1. Model description

The mechanistic, deterministic, simulation model DAISY is open software, which simulates water, C and N dynamics in the soil–plant–atmosphere system. The model consists of more than 100 submodels for simulating soil–vegetation–atmosphere transfer processes, soil physical processes like soil water and solute movement, and soil temperature; organic matter turnover resulting in mineralization and immobilization of soil solution nitrate and ammonium; crop growth and physiology including different submodels of photosynthesis and radiation distribution in the canopy; along with a detailed system of management operations at field scale. Simulations are performed by combining relevant submodels and setting a number of parameters describing the soil, crop, climatic conditions and management operations. For the processes involved in the simulation, mass balances can be calculated. The source code as well as the original documentation (Hansen et al., 1990) can be downloaded from the homepage (DAISY, 2007). In DAISY, DOM is quantified with respect to C and N, which is referred to as dissolved organic C (DOC) and dissolved organic N (DON), respectively. Each horizon defined in the DAISY set-up is parameterized separately according to soil texture, C and N contents, and Fe and Al contents in the set-up file. The transport of DOM in the entire soil profile is calculated by solving the convection dispersion equation.

2.1.1. Biological turnover of organic matter and formation of DOM

An overview of the individual soil organic matter pools in DAISY and the dynamics between the pools are described in Fig. 1. Further information of the organic

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