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A model to calculate effects of atmospheric deposition on soil acidification, eutrophication and carbon sequestration

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ABSTRACT

Triggered by the steep decline in sulphur deposition in Europe and North America over the last decades, research and emission reduction policies have shifted from acidification to the effects of nitrogen (N) deposition and climate change on plant species diversity and carbon (C) sequestration in soils and biomass. Consequently, soil-ecosystem models need to include detailed descriptions of C and N processes, and ideally provide output that link to plant species diversity models. We describe an extension of the Very Simple Dynamic (VSD) model, called VSD+, which includes an explicit description of C and N turnover. Model simulations for three forest stands, which differ in N deposition and soil C/N ratios, show that VSD+ can well predict both trends and absolute values of NO_3 and NH_4 concentrations in soil and stream waters, soil C/N ratios and pH, which makes VSD+ suitable for providing input for plant species diversity models.

Software availability

Name of software: VSD+ (version 1.4)
Developers: Luc Bonten, Gert Jan Reinds, Maximilian Posch
Contact address: Alterra-Wageningen UR, P.O. Box 47, 6700 AA Wageningen, The Netherlands, E-mail: gertjan.reinds@wur.nl
Year first available: 2015 for version 1.4 (2012 for version 1.0)
Required software: Windows
Program Language: Intel Visual Fortran (GUI: Embarcadero C++ Builder)
Availability and cost: downloadable for free from http://wge-cce.org/Methods_Data/The_VSD_suite_of_models

1. Introduction

Since ‘acid rain’ became an issue in the late 1970s and early 1980s, numerous models for have been developed to simulate the processes involved in the acidification of soils and surface waters, such as the Enhanced Trickle Down (ETD) model (Nikolaidis et al., 1989), the Integrated Lake-Watershed Acidification Study (ILWAS) model (Gherini et al., 1985) and the Birkeness model (Christophersen et al., 1982). These models cover a wide spectrum of applications and objectives. Many of them are research models that were developed for certain projects and/or sites for which detailed measurements were available (e.g. Tiktak and Van Grinsven, 1995). While developing and evaluating such models is very important to advance our understanding of individual processes and their interactions, they are often not suitable for regional applications, as they require detailed input data not readily available on a regional scale.

Since the acidification problem is caused by transboundary air pollutants, primarily from emissions of sulphur dioxide (SO_2), travelling over large distances, common abatement measures (for Europe) were negotiated in subsidiary bodies of the 1979 UNECE Convention on Long-range Transboundary Air Pollution. It was agreed at an early stage that assessments of emission reductions should be effects-based, i.e. based on the sensitivity of ecosystems to the deposition of sulphur (S) and nitrogen (N) (e.g. Hettelingh et al., 2007). This sensitivity was assessed using so-called critical loads, i.e. steady-state deposition levels below which ‘significant harmful effects’ do not occur (see e.g. De Vries et al., 2015a; CLRTAP, 2004).

In parallel with the steady-state modelling of critical loads, simple dynamic models describing soil and surface water acidification emerged, designed to be easily applicable at many sites,

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having only modest input data requirements and paying attention to the ease (and speed) of use. The most widely used are the catchment model MAGIC (Cosby et al., 2001), and the soil models SAFE (Warfvinge et al., 1993) and the Very Simple Dynamic (VSD) model (Posch and Reinds, 2009). Since their inception, these models have been continuously developed, compared to observations at numerous intensively monitored sites (e.g. Forsius et al., 1998; Tominaga et al., 2010), albeit mostly in Europe, and also played an important role in providing information on temporal dynamics. Dynamic soil acidification models do not only allow rapid scenario analyses, but also the calculation of target loads, i.e. deposition targets which result in a desired chemical condition in the soil (solution) in a specified future year (e.g. Jenkins et al., 2003).

As a consequence of the steep decline of S emissions during the last decades (e.g., Vestreng et al., 2007), the focus in research and policy has shifted from acidification to the various effects of N deposition. The emissions of oxidised N have also declined in most of Europe over the last two decades (e.g., Rafaj et al., 2014), albeit at a slower pace, whereas reduced N emissions have even increased in parts of Europe, resulting in total N becoming the dominant pollutant (Amann et al., 2013). Furthermore, climate change issues and the concern for biodiversity have led to a refocussing of the effects-oriented work in support of European emission reduction policies. Concerns for the effects of surplus N and climate change on the diversity of plant species (e.g. Bobbink et al., 2010; Sutton et al., 2014) and the sequestration of carbon (C) in the soils and biomass (e.g. Hyvönen et al., 2007; De Vries et al., 2014) have prompted model developers to enhance their models with more detailed descriptions of C and N processes, and to provide output variables needed for downstream plant species diversity models. For example, the SAFE model has expanded into the model ForSAFE (Wallman et al., 2005) and a more detailed description of N and C cycling has been added to MAGIC (Oulehle et al., 2012); and the extension of the VSD model is subject of this paper.

In this paper we describe an extension of the VSD model (Posch and Reinds, 2009), called VSD+, that incorporates an enhanced description of changes of C and N pools and their interactions, following the RothC model (Coleman and Jenkinson, 2014). Here, we only describe the processes and equations that go beyond those of the basic VSD model as described by Posch and Reinds (2009). In addition, we evaluated the enhanced model, using data from three sites with widely differing combinations of N deposition and present-day soil C/N ratios. In the Supplementary Information we describe a Graphical User Interface for the VSD+ model (VSD+Studio) and its use for single-site calibration and application. In addition, we describe two auxiliary programs that can be used for pre-processing climate data and related parameters for use in the VSD+ model (the MetHyd model) and for deriving N uptake and litterfall data from a simple growth model (the GrowUp model).

2. Material and methods

2.1. Model description

The VSD+ model includes an explicit description of organic C and N turnover, whereas in the VSD model (Posch and Reinds, 2009) N immobilisation depends on the N availability and C sequestration subsequently depends on the N immobilisation rate, controlled by user-prescribed C/N ratios. Most other processes are similar to the original VSD model as described by Posch and Reinds (2009). We included a Ca and Mg carbonate equilibrium, which means that VSD+ can also be used for calcareous soils. A comprehensive description of the equilibrium and elemental mass balance equations is given below, and a detailed description can be found in Posch and Reinds (2009).

2.1.1. Equilibrium and mass balance equations

The VSD+ model is a single-layer model which consists of charge and mass balances to calculate changes in pH and element concentrations in the soil solution and an organic C and N model. At every time step the charge balance (Eq. (1)) determines the proton concentration, i.e. pH, in the soil solution from the concentrations of other elements and dissolved organic anions:

$$\left[H^+\right] = \left[SO_4^{2-}\right] + \left[NO_3^-\right] + \left[Cl^-\right] + \left[HCO_3^-\right] + \left[Org^-\right] - \left[Ca^{2+}\right] - \left[Mg^{2+}\right] - \left[K^+\right] - \left[Na^+\right] - \left[Al^{3+}\right] - \left[NH_4^+\right] \tag{1}$$

The changes in the concentrations of elements follow from a mass balance for the individual elements (Eq. (2)). This equation describes the change in the total amount of an element over time in the soil. The total amount (eq m^{-2}) is the sum of the amounts of the element in the soil solution and in the soil solid phase.

$$\frac{d}{dt}([X]\cdot\theta\cdot z + X_s\cdot\rho\cdot z) = X_{in} - \Phi\cdot[X] \tag{2}$$

where $[X]$ (eq m^{-3}) is the concentration of an element in the soil solution, X_s (eq kg^{-1}) is the concentration in the solid phase, θ (m^3 m^{-3}) is soil moisture content, z (m) is the thickness of the soil layer in the calculation, normally the rooting zone, ρ (kg m^{-3}) is the bulk density of the soil, X_{in} (eq m^{-2} yr^{-1}) is the sum of all sources minus sinks, and Φ (m yr^{-1}) is the water discharge (precipitation surplus). For Al, HCO_3^- and organic acids no mass balance is considered; their supply is assumed to be unlimited, and they are calculated from equilibrium equations with $[H^+]$. For calcareous soils we also assume an infinite supply of Ca and Mg (see Section 2.1.2). The left-hand side of Eq. (2) includes the total amount of an element in the soil (expressed in eq m^{-2}) which is the sum of the element in the soil solution and in the soil solid phase. Complexation of SO_4, NO_3, NH_4, Na and Cl by the soil solid phase are not modelled in VSD+, and therefore their solid phase concentrations are zero and their total amount equals the amount in soil solution. The base cations Ca, Mg, K in the solid phase are sorbed at the exchange complex (Eq. (3)):

$$X_s = E_X\cdot CEC \tag{3}$$

where E_X is the equivalent fraction of base cation X at the exchange complex, and CEC (eq kg^{-1}) is the cation exchange capacity. In VSD+ sorption of the base cations is calculated by exchange between the solid phase and the soil solution with Al, H. The Gaines–Thomas model or the Gapon model can be chosen by the user to model cation exchange. For the Gapon model Ca, Mg and K are summed as Bc, where two K^+ ions are treated as one divalent ion. For the Gaines–Thomas model sorption of Ca, Mg and K can be calculated separately, albeit that the exchange constants are the same for all three base cations. Aluminium concentrations in soil solution are calculated from the equilibrium dissolution of Al hydroxides.

The right-hand side of Eq. (2) includes the sinks and sources of elements, as well as element leaching as a consequence of water discharge. Sinks and sources in VSD+ are deposition (all elements), weathering (Ca, Mg, K, Na), input from litterfall (Ca, Mg, K), uptake by plants (Ca, Mg, K, NH_4, NO_3), mineralisation (NH_4), nitrification (NH_4, NO_3) and denitrification (NO_3). VSD+ includes rate-limited