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# Comparison of model concepts for nutrient availability and soil acidity in terrestrial ecosystems

KWR Watercycle Research Institute

WAGENINGEN UNIVERSITY & RESEARCH

# Comparison of model concepts for nutrient availability and soil acidity in terrestrial ecosystems

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# Abstract

STOWA heeft het initiatief genomen om samen met een aantal partijen een klimaatrobuuste Waterwijzer Natuur (WWN) te ontwikkelen. Een instrument dat de effecten van klimaatverandering en het waterbeheer op de terrestrische vegetatie van natuurgebieden dient te kunnen berekenen. Klimaatverandering zal vooral gevolgen voor natuurlijke vegetaties hebben via veranderingen in de waterbalans. Die veranderingen werken namelijk door op de bodemtemperatuur en de hoeveelheid vocht, zuurstof en nutriënten die voor de planten in het wortelmilieu beschikbaar zijn. Klimaatverandering noopt dan ook tot het stellen van enkele essentiële vragen, zoals:

- Welke maatregelen zijn er nodig om natuurdoelen in de toekomst zeker te stellen?
- Welke alternatieve doelen kunnen we overwegen als in het verleden vastgestelde natuurdoelen niet meer haalbaar blijken te zijn onder een veranderend klimaat?
- Waar liggen straks, in het klimaat van de toekomst, de beste kansen voor het creëren van hotspots van biodiversiteit?

Dit rapport geeft een overzicht van de overeenkomsten en verschillen van de wijze waarop PROBE (KWR) en VSD+ (WEnR) de nutriëntenbeschikbaarheid en zuurgraad in (half)natuurlijke terrestrische ecosystemen voorspellen in afhankelijkheid van milieu, (vnl. atmosferische depositie), klimaat (vnl. temperatuur en neerslag) en waterbeheerscenario's.

De belangrijkste conclusies zijn:

- PROBE is sterk in de berekening van stikstofbeschikbaarheid en hanteert een meer procesmatige aanpak dan VSD+ om de effecten van bepaalde milieufactoren te modelleren. Verder bieden de fijne ruimtelijke en temporele resoluties van dit model de mogelijkheid om seizoeneffecten, de invloed van regenwaterlenzen, weersextremen en beheersmaatregelen op een procesmatige basis mee te nemen, wat vooral voor de bodem-pH in natte gebieden van belang is. De pH module van PROBE is echter niet robuust voor alle vegetatie-bodem combinaties en dient te worden verbeterd of aangepast.
- VSD+ is sterk in de berekening van zuurgraad (pH), omdat het een volledige ionenbalans bevat op basis waarvan het effect van alle mogelijke zuur-producerende en zuur-bufferende processen op de pH wordt meegenomen. Het model is echter zwak in natte systemen omdat redoxprocessen niet zijn meegenomen. Dit zou moeten worden toegevoegd met het oog op toepasbaarheid in natte systemen.
- In beide modellen is de fosfaatbeschikbaarheid nog niet goed ingebracht. Dit kan essentieel zijn voor een goede voorspelling van effecten van maatregelen

Daarnaast geeft dit rapport een overzicht van de belangrijkste datasets die aanwezig zijn voor het parametriseren en valideren van beide modellen.

# Uitgebreide samenvatting

## *S1 Inleiding*

Waterbeheerders hebben als taak op een verantwoorde wijze om te gaan met de beschikbare hoeveelheid water van de juiste kwaliteit. Om dat goed te kunnen doen is kennis nodig over de waterverdeling op verschillende ruimtelijke schaalniveaus, variërend van een enkel perceel tot het gehele land. Bovendien dienen waterbeheerders inzicht te hebben in de gevolgen van het door hen gevoerde beheer. In het landelijk gebied zijn het vooral de landbouw, de natuur en de drinkwaterbedrijven die hiervan afhankelijk zijn.

De beoordeling van gevolgen voor de landbouw gebeurde tot nu toe met instrumenten, zoals de HELP-tabellen, die zijn gebaseerd op inmiddels verouderde kennis en die ongeschikt zijn voor klimaatprojecties. STOWA heeft daarom het initiatief genomen om samen met een aantal partijen een klimaatrobuuste beoordelingssystematiek voor de landbouw te laten ontwikkelen. Daarnaast heeft STOWA het initiatief genomen om ook een Waterwijzer Natuur (WWN) te ontwikkelen. Een instrument dat de effecten van klimaatverandering en het waterbeheer op de terrestrische vegetatie van natuurgebieden dient te kunnen berekenen. In beide waterwijzers zijn processen die door klimaatverandering worden beïnvloed zo goed mogelijk nagebootst. Door deze procesbenadering zijn ze ook geschikt voor klimaatprojecties en extreme weercondities, in tegenstelling tot instrumenten die vooral gebaseerd zijn op empirische relaties ontleend aan het recente klimaat en deskundigenoordeel.

De ontwikkeling van de WWN is opgenomen in de Landelijke Kennisagenda Zoetwater die door het Bestuurlijk Platform Zoetwater is vastgesteld. Samen met de Waterwijzer Landbouw kan de WWN worden beschouwd als een belangrijk instrument voor de onderbouwing van een Deltaplan Zoetwater fase 2 (2022 – 2027). De ambtelijke IPO-vertegenwoordigers in het Deltaplan Zoetwater hebben aangegeven dat de provincies een logische partij vormen om de ontwikkeling van de WWN mogelijk te maken. Dit onderzoek is daar het gevolg van.

In Nederland is natuur ruimtelijk gepland: er zijn voor alle natuurterreinen doelen vastgesteld. Vaak zijn die natuurdoelen wettelijk vastgelegd, bijvoorbeeld in Europees verband (Habitatrichtlijn/Natura 2000, Kaderrichtlijn Water). Verschillende organisatie hebben hierbij hun taken en verantwoordelijkheden. Provincies zijn verantwoordelijk voor natuurbehoud en –ontwikkeling (het Nationaal Natuurnetwerk, voorheen EHS). Hydrologische voorwaarden creëren is daarvoor een belangrijke maatregel. Waterschappen geven uitvoering aan hydrologische herstelmaatregelen.

Het klimaat van Nederland verandert echter, en dat heeft consequenties voor de haalbaarheid van natuurdoelen, zoals de PBL-studie ‘effecten van klimaatverandering in Nederland: 2012’ laat zien. Klimaatverandering zal vooral gevolgen voor natuurlijke vegetaties hebben via veranderingen in de waterbalans. Die veranderingen werken namelijk door op de bodemtemperatuur en de hoeveelheid vocht, zuurstof en nutriënten die voor de planten in het wortelmilieu beschikbaar zijn. Klimaatverandering noopt dan ook tot het stellen van enkele essentiële vragen, zoals:

- Welke maatregelen zijn er nodig om natuurdoelen in de toekomst zeker te stellen?
- Welke alternatieve doelen kunnen we overwegen als in het verleden vastgestelde natuurdoelen niet meer haalbaar blijken te zijn onder een veranderd klimaat?
- Waar liggen straks, in het klimaat van de toekomst, de beste kansen voor het creëren van hotspots van biodiversiteit?

Op dit moment ontbreekt het de waterbeheerder en beleidsmaker aan een praktisch instrument om dergelijke vragen te beantwoorden. Het gebrek hieraan kan leiden tot een beleid en beheer dat onvoldoende is afgestemd op de natuur, en op een navenant suboptimale besteding van middelen voor de natuur. Het is relevant voor zowel de overheid als voor gebiedspartijen om te weten of een investering in de natuur langdurig resultaat oplevert, of dat er op termijn een nieuwe investering nodig zal zijn.

Daarom hebben STOWA, het Ministerie van EZ, Rijkswaterstaat-WVL en de stichting Kennis voor Klimaat door drie onderzoeksinstituten een verkennend onderzoek laten verrichten waarin verschillende modelconcepten met elkaar werden vergeleken. Eén van de conclusies uit dit onderzoek komt erop neer dat bestaande computermodellen niet geschikt zijn voor klimaatprojecties, omdat ze zijn gebaseerd op indirecte relaties tussen standplaats en vegetatie die bovendien ontleend zijn aan het klimaat van de vorige eeuw. Dat geldt bijvoorbeeld voor het in nationale beleidsstudies gebruikte model DEMNAT, waarmee alleen voor het huidige klimaat kan worden beoordeeld hoe per vierkante kilometer de relatieve soortenrijkdom van een 18-tal ecosysteemtypen verandert wanneer de waterstand daalt of stijgt. Met hogere temperaturen, een langer groeiseizoen, meer extreme neerslagbuien, afgewisseld door langdurige perioden van droogte, kunnen deze modellen niet omgaan. Daarnaast werd gesignaleerd dat het modelleren van de zuurgraad en nutriëntenstatus van de bodem de zwakste schakel is bij het modelleren van effecten op de vegetatie.

Op basis van deze bevindingen zijn de volgende vervolgstappen voorgesteld:

- Gebruik het model PROBE als basis voor de ontwikkeling van de WWN.
- Besteed vooral aandacht aan de zwakste modelonderdelen: de berekening van de zuurgraad en nutriëntenstatus van de bodem.
- Zorg voor een gebruiksvriendelijke toepassing/schil.

Dit onderzoek gaat in op het tweede punt. Financiers en andere betrokken partijen bij het onderzoek zijn:

- STOWA
- Deltaprogramma Zoetwater (Ministerie van Infrastructuur en Milieu)
- Ministerie van Economische Zaken
- Planbureau voor de Leefomgeving
- Provincies Gelderland, Utrecht en Noord-Brabant
- Waterschap Aa & Maas en Waterschap Vechtstromen
- Kennisprogramma Lumbricus
- Natuurmonumenten en Staatsbosbeheer
- KWR en WEnR

Mondiaal gezien zijn er behoorlijk wat modellen in omloop waarmee de zuur- en nutriëntendynamiek gemodelleerd kunnen worden. In deze analyse beperken wij ons echter tot twee modellen waarmee met name in Nederland ervaring is opgedaan. Het gaat hierbij om de modelversies van PROBE (bestaande uit de modellen SWAP, CENTURY en ORCHESTRA) ontwikkeld door het KWR en het VSD+ model, gekoppeld aan GrowUp en SUMO, ontwikkeld door WEnR (hierna genoemd VSD+).

## *S2 Resultaten*

In grote lijnen zijn de modellen PROBE en VSD+ vergelijkbaar. Beide modellen hebben als doel standplaatsfactoren, zoals vochtgehalte, zuurgraad en nutriëntenbeschikbaarheid in (half)natuurlijke terrestrische ecosystemen te voorspellen in afhankelijkheid van milieu (vnl. atmosferische depositie), klimaat (vnl. temperatuur en neerslag) en waterbeheerscenario’s. Het belangrijkste verschil tussen beide modellen is dat het model VSD+ qua procesformulering eenvoudiger en minder gedetailleerd is dan het model PROBE.

### *S2.1 Modelvergelijking*

#### *Structuur*

In onderstaande figuur is een overzicht gegeven van de structuur en de relaties tussen de onderliggende modules van beide modellen.

Zo worden, om de rekensnelheid te verhogen,  in PROBE-2.1 (Witte *et al.*, 2015) de standplaatsfactoren berekend met metarelatiesdie zijn afgeleid van het agrohydrologische model SWAP (voor bodemvocht) en het bodemmodel uit CENTURY (voor N beschikbaarheid). In PROBE-2.2 (Cirkel *et al.*, 2016a) is de bodem-pH als factor toegevoegd door koppeling met het bodemchemische model ORCHESTRA in combinatie met het hydrologische model SWAP. Ten slotte zijn in PROBE-3 (Fujita *et al.*, 2016) het model SWAP, CENTURY-bodemmodule en de CENTURY-plantmodule dynamisch gekoppeld om zowel het bodemvocht als de N-beschikbaarheid te berekenen. In PROBE-3 wordt de pH echter niet dynamisch berekend, maar benaderd op basis van empirische relaties gebaseerd op Aggenbach *et al.* (2013a) en Stuyfzand (2010). PROBE-2.1 is toegepast voor de natte natuur in twee beekdalen de ‘Baakse Beek’ (Witte *et al.*, 2015) en de ‘Tungelrooyse Beek’ (Van der Knaap *et al.*, 2015; Van der Knaap *et al.*, submitted), terwijl PROBE-3 toegepast is op kustduinen en een landbouwgewas (Fujita *et al.*, 2016). Om de verschillende modelversies op nationale schaal te kunnen toepassen zijn reprofuncties afgeleid voor diverse Nederlandse bodemtypes. Voor versies 2.2 en 3 is dat maar ten dele gelukt. PROBE-2.1 heeft een gebruikersvriendelijk userinterface, wat wordt beschouwd als een prototype van de WWN. Via de interface kunnen gebruikers diverse klimaat- en hydrologie-scenario’s selecteren voor toepassing op landschapsschaal, waarbij gebruik gemaakt wordt van ruimtelijk expliciete geografische informatie op 25 m × 25 m resolutie. PROBE-3, daarentegen, is voorzien van eenvoudige userinterface die is bedoeld voor toepassingen op standplaatsniveau.

In dit rapport richten we ons op de combinatie PROBE-3 (voor dynamische hydrologie en N beschikbaarheid en relatie met de vegetatie) en PROBE-2.2 (voor dynamische pH). In Figuur S1 is de onderlinge relatie tussen de modules aangegeven. Als tijdstap wordt een dag gehanteerd en de eendimensionale ruimtelijke schaal bestaat uit bodemlaagjes van 1 cm. De totale gemodelleerde bodemlaag bestrijkt 6 m en de tijdhorizon 1 jaar tot enkele decennia.

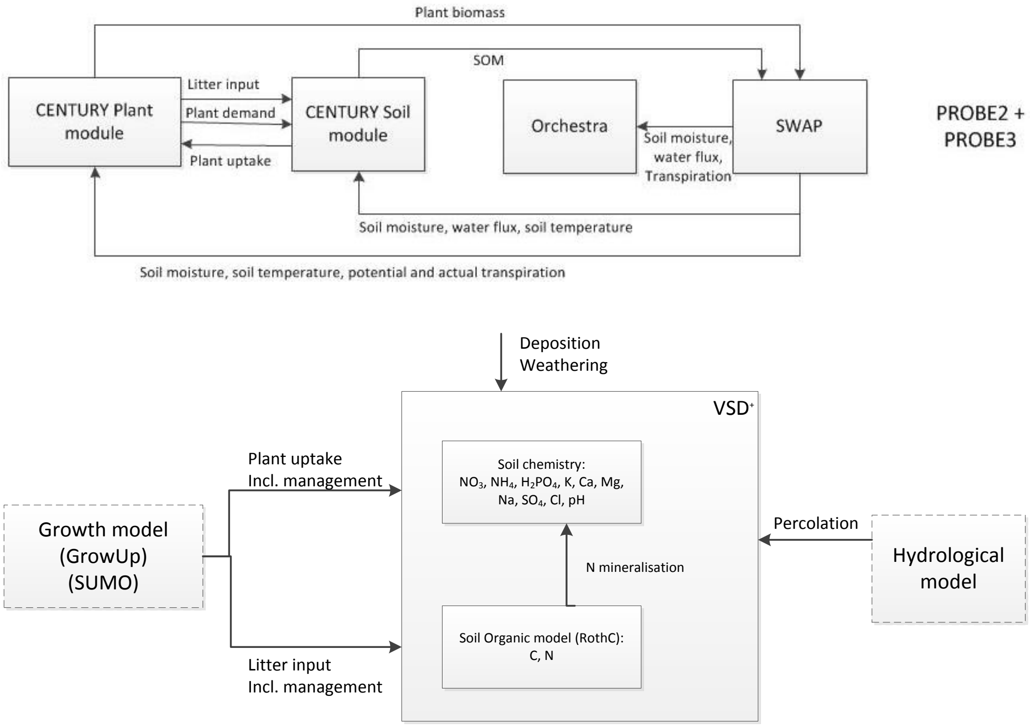
Het VSD$^{+}$ model (Bonten *et al.*, 2016) berekent zowel de dynamiek als de bodemvochtconcentratie van $SO_4$, $PO_4$, Ca, Mg, K, Na, Cl, $NO_3$ en $NH_4$ de C/N ratio en de pH. Dit maakt het model geschikt voor het aanleveren van de benodigde standplaatsfactoren ten behoeve van plantendiversiteit modellen, zoals de vegetatiemodule van PROBE.

Het VSD$^+$ model bestaat uit één bodemcompartiment en rekent standaard met een tijdstap van 1 jaar. Het model berekent zowel de pH als de C- en N-dynamiek en is met name bedoeld voor toepassingen op regionale schaal. Het model bevat alle belangrijke zuurproducerende en zuurneutraliserende processen zoals mineraalverwering, kationenomwisseling, (de)nitrificatie, nutriëntopname en mineralisatie. De pH wordt berekend uit de ladingsbalans in de bodemoplossing. Voor de dynamiek van C- en N-pools in organische stof wordt gebruik gemaakt van het model RothC (Coleman & Jenkinson, 2014). Het RothC is volledig geïntegreerd met het VSD+ model. De jaarlijkse interacties tussen de bodem-pH enerzijds en mineralisatie en (de)nitrificatie anderzijds, zijn beschreven middels reductiefuncties.

Voor de waterbalans maakt het model gebruik van de invoer van een hydrologisch model. Dit kan ieder gewenst model zijn, bijv. SWAP. Dit geldt ook voor de relatie met de vegetatie. Bij VSD+-toepassing wordt veelal gebruik gemaakt van het model GrowUp. Deze module simuleert planten(bos)groei, strooiselproductie en nutriëntopname. Daarnaast wordt gebruik gemaakt van het vegetatie-successiemodel SUMO, waardoor het mogelijk is effecten van vegetatiebeheer (zoals begrazen, maaien, afplaggen) te simuleren. Zie Figuur S1 voor de onderlinge relatie tussen de modules.

Het model heeft slechts een beperkte hoeveelheid aan input nodig, omdat veel gegevens reeds aanwezig zijn. Dit geldt voor geheel Nederland. De rekentijd van het model is minimaal (< 1 minuut bij toepassing voor geheel Nederland op een 250m × 250m resolutie). Het model is voorzien van een gebruiksvriendelijke grafische user interface (GUI). Deze GUI stelt de gebruiker eenvoudig in staat om zowel (Bayesian) kalibraties uit te voeren als scenario's door te rekenen.

FIGUUR S1 RELATIE TUSSEN DE DIVERSE MODULES (PLANT, BODEMORGANISCHE STOF, HYDROLOGIE EN CHEMIE) IN PROBE (BOVEN) EN VSD+-(ONDER).

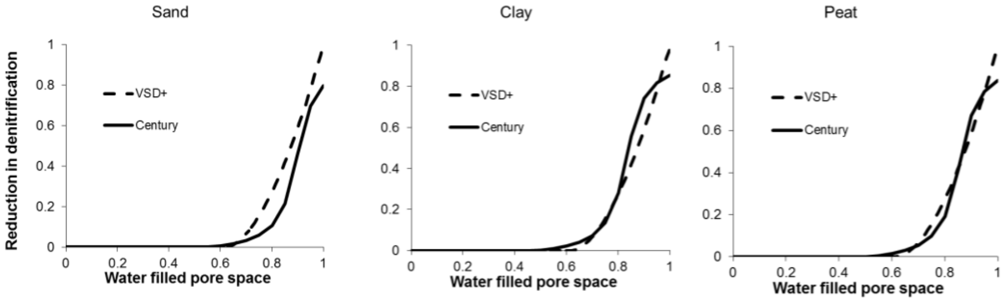


### *Reductie-functies*

Naast een vergelijk op hoofdlijnen, zoals type processen en mate van detail is er ook een gedetailleerde vergelijking uitgevoerd van de functies waarmee het verband tussen de abiotische factoren, zoals bodemvocht, temperatuur, textuur, pH, CN-ratio en N-beschikbaarheid enerzijds en mineralisatie, (de)nitrificatie, groei, en N-gehalte van de vegetatie anderzijds.

In veel gevallen zijn de reductiefuncties, zoals gebruikt in beide modellen, vergelijkbaar. Zie bijv. Figuur S2 waarin de gehanteerde reductiefuncties voor de relatie vocht-denitrificatie worden getoond. Sommige reductie functies zijn slechts in één van beide modellen opgenomen, bijvoorbeeld voor het effect van bodemvocht op plantensterfte en het pH-effect op denitrificatie (zie Figuur S3).

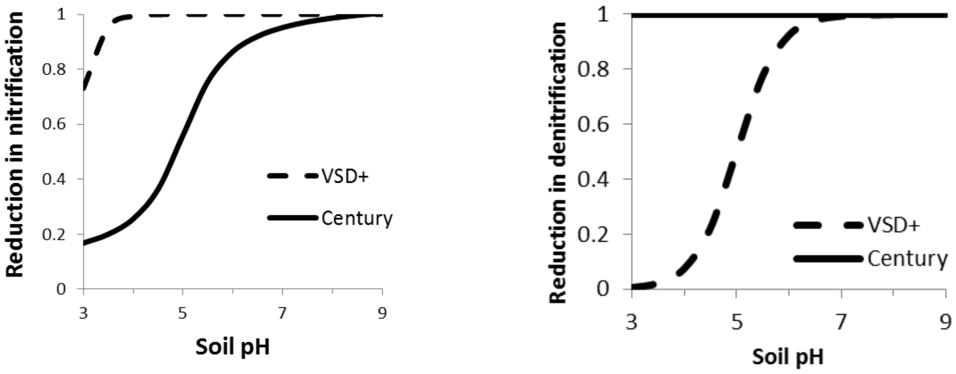
FIGUUR S2 EFFECT VAN VOCHT OP DENITRIFICATIE IN PROBE EN VSD+ VOOR ZAND (‘BOUWSTEEN’ B1), KLEI (‘BOUWSTEEN’ B11) EN VEEN (‘BOUWSTEEN’ B15).



Indien daar aanleiding toe is zijn de reductiefuncties vrij eenvoudig aan te passen en ontbrekende relaties vrij eenvoudig toe te voegen. Dit vereist geen ingrijpende wijzigingen in de modelstructuur. Een lastig punt hierbij is overigens, dat het niet altijd mogelijk is om een objectieve keuze te maken op een reductiefunctie door het ontbreken van de juiste proceskennis.

Er zijn echter ook relaties in beide modellen die in sterke mate van elkaar verschillen, zoals het effect van de CN-ratio van organische stof op de N-beschikbaarheid en het effect van pH op (de)nitificatie (zie figuur S3).

FIGUUR S3 EFFECT VAN PH OP NITRIFICATIE IN CENTURY EN VSD+ (LINKS) EN OP DENITRIFICATIE IN VSD+ (RECHTS).



*Definities van nutriëntenbeschikbaarheid in relatie tot vegetatie-effecten*

Naast de rol van N speelt ook fosfor (P) een belangrijke rol. Wij zijn dan ook van mening dat voor het modelleren van nutriëntenbeschikbaarheid niet alleen de N-beschikbaarheid, maar ook de P-beschikbaarheid dient te worden beschouwd.

Vanuit het oogpunt van de vegetatie nemen we aan dat de mineralisatiesnelheid van N en/of P een representatievere benadering voor de nutriëntenbeschikbaarheid is dan de totaal gehaltes of extraheerbare hoeveelheden N en/of P in de bodem. Een mineralisatieflux betreft immers de resultante van de beschikbare hoeveelheid N en/of P en de mate waarin deze vrijkomt in afhankelijkheid van omgevingsfactoren zoals temperatuur en vocht. Dit wordt ondersteund door onderzoek van Fujita *et al.* (2013). Daarom wordt voorgesteld om vooralsnog uit te gaan van de netto mineralisatieflux als maat voor de voedselrijkdom van de bodem. Echter, naast de netto mineralisatie is met name ook de toevoer van N via atmosferische depositie, grondwaterstroming en via N-fixatie door bodemorganismen van belang, maar ook de afvoer als gevolg van denitrificatie. In geval van P is daarnaast ook de toevoer via verwering (en mogelijk via sorptie) en de eventuele aanvoer via kwelwater van belang. Dit resulteert in de volgende werkdefinities van N- en P-beschikbaarheid:

N-beschikbaarheid = netto N mineralisatie + atmosferische N depositie + N-fixatie – denitrificatie + N-kwelwater

P-beschikbaarheid = netto P mineralisatie + atmosferische P depositie + P sorptie + P verwering + P-kwelwater

We hebben een aantal datasets geselecteerd aan de hand waarvan de modellen nader getest en met elkaar kunnen worden vergeleken en gevalideerd. In totaal zijn negen datasets geselecteerd die gebruikt kunnen worden voor de parametrisatie op landelijke schaal. Met het oog op validatie zijn tien monitoringreeksen geïnventariseerd, waarvan er een viertal geschikt lijkt om te worden gebruikt voor het uitvoeren van een modelvergelijking en validatie. Een manco is wel dat het merendeel van deze datasets zich richt op de drogere terrestrische ecosystemen, waardoor de nattere en anoxische systemen onvoldoende zijn vertegenwoordigd.

### *S2.2 Sterke en zwakke punten van beide modellen*

Op basis van de uitgevoerde modelvergelijking komen we tot de volgende sterke en zwakke punten:

*Sterke punten PROBE*

- Een procesmatige en consistente beschrijving van nutriëntenlimitatie en het effect van C:N:P stoichiometrie op plantengroei en mineralisatie.
- Dynamische terugkoppeling tussen plant, bodem en hydrologie.
- Expliciete modellering van het effect van de pH beïnvloeding via grondwater.
- Meerlagenmodel, waardoor het mogelijk is om de verticale gradiënt in bodemchemie en bodemvochtconcentratie te modelleren.
- Bovendien een kleine rekentijdstap waardoor seizoeneffecten, de invloed van regenwaterlenzen, weersextremen en beheersmaatregelen kunnen worden meegenomen.

*Zwakke punten PROBE*

- Vrij complex en vraagt om veel input data.
- Lange rekentijden.
- pH module is niet gekoppeld met de bodemorganische-stofmodule.

*Sterke punten VSD+*

- Relatief eenvoudig en vraagt om relatief weinig input data.
- Bevat alle macro-ionen (volledig ladingsbalans).
- Dynamische interactie tussen pH en biochemische processen.
- In combinatie met SUMO is het mogelijk om interacties tussen bodem en vegetatiegroei en de effecten van vegetatiebeheer zoals plaggen en maaien te simuleren.
- Rekent snel.
- Eenvoudig toe te passen als gevolg van relatie met de nationale databases en gebruiksvriendelijke user interface.

*Zwakke punten VSD+*

- Hanteert een constante C:N ratio voor iedere organische-stofpool.
- Bevat geen P-mineralisatie en chemische interactie is beperkt tot direct P sorptie evenwicht met een labiele P pool.
- Combinatie met SUMO is niet gevalideerd en vraagt om vrij veel aanvullende input data.
- Seizoeneffecten zijn niet expliciet mee te nemen als gevolg van een jaarlijkse tijdstap.
- Bevat geen redoxprocessen.

## *S3 Conclusies en aanbevelingen*

### *S3.1 Conclusies*

- PROBE is sterk in de berekening van stikstofbeschikbaarheid en hanteert een meer procesmatige aanpak dan VSD+ om de effecten van bepaalde milieufactoren te modelleren. Verder biedt de kleine rekentijdstap en opdeling in vele bodemlaagjes de mogelijkheid om seizoeneffecten, de invloed van regenwaterlenzen, weersextremen en beheersmaatregelen op een procesmatige basis mee te nemen, wat vooral voor de bodem-pH in natte gebieden van belang is. De pH module van PROBE is echter niet robuust voor alle vegetatie-bodem-combinaties en dient te worden verbeterd of aangepast.
- VSD+ is sterk in de berekening van zuurgraad (pH) omdat het een volledige ionenbalans bevat op basis waarvan het effect van alle mogelijke zuur-producerende en zuur-

bufferende processen op de pH wordt meegenomen. Het model is echter zwak in natte systemen omdat redox-processen niet zijn meegenomen. Dit zou moeten worden toegevoegd met het oog op toepasbaarheid in nattere systemen.

- In beide modellen is de fosfaatbeschikbaarheid nog niet goed ingebracht. Dit kan essentieel zijn voor een goede voorspelling van effecten van maatregelen.
- Om objectief vast te kunnen stellen wat de optimale balans is in de mate van modeldetail en mate van interactie tussen de processen, dienen beide modellen te worden toegepast op één of meerdere van de geselecteerde datasets. Dit zal in fase 2 worden uitgevoerd.

### *S3.1 Aanvelingen*

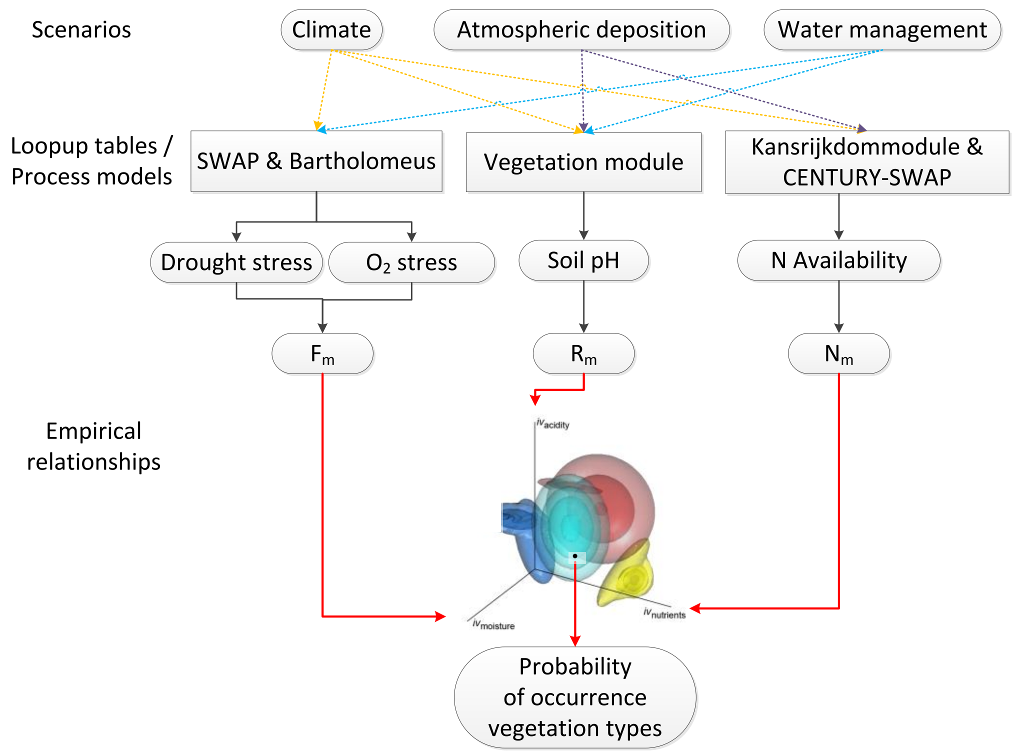
- Zuurgraad: verbeter de beschrijving van de kationomwisseling en daarmee de relatie pH-basenverzadiging die essentieel is voor de voorspelling van de zuurgraad in het pH traject van 4.5-6.5. Bovendien dient beter rekening te worden gehouden met de invloed van kwelwater.
- N-beschikbaarheid: verbeter de onderbouwing van de relaties tussen de stikstoftransformaties (mineralisatie, nitrificatie en denitrificatie) in afhankelijkheid van het vochtgehalte en de zuurgraad (pH). Deze zijn essentieel voor een robuuste voorspelling van N-beschikbaarheid en de $NO_3$-uitspoeling.
- P-beschikbaarheid: betrek de naast N-beschikbaarheid ook P-beschikbaarheid om de effecten op de vegetatie in beeld te brengen. Probeer hiervoor een relatie af te leiden tussen beschikbaar (geadsorbeerd) fosfaat in de bodem (en in de bodemoplossing) en biomassa-productie.

# Contents

# 1 Introduction

The WaterWijzer Natuur (WWN) is meant to test and predict the occurrence probability of vegetation types, both under current and forecasted climate conditions. Whether or not vegetation types (phyto-sociological associations, nature target types, habitat types) can persist where they occur or have been planned, is tested on the basis of three site factors, i.e. moisture regime, nutrient availability, and soil acidity (Figure 1).

FIGURE 1 SCHEMATIC REPRESENTATION OF THE WATERWIJZER NATUUR (WWN)



Reliable estimates of these three site factors in view of changes in climate, groundwater levels and atmospheric deposition, requires a process based modelling approach. Based on the work of Bartholomeus et al. (2008; 2011) and Bartholomeus & Witte (2013), the effect of soil moisture has been adequately modelled (Witte *et al.*, 2015). The modelling of nutrient availability and acidity, however, needs substantial improvement.

The knowledge on vegetation effect modelling in the Netherlands is distributed amongst various research institutes (i.e. KWR, Wageningen Environmental Research (WEnR) and PBL) in the Netherlands, being an inefficient and unwanted situation. Therefore, STOWA, the Ministry of Economic Affairs, Ministry of Transport-WVL and the Knowledge for Climate Foundation decided to combine the research forced of the involved institutes on this topic. In a previous project a pilot study the different model concepts at the research institutes were compared (Van Ek *et al.*, 2014). One of the conclusions of this research was that the existing models are not suitable for climate projections, because they are based on indirect relationships between habitat and vegetation using the climatic situation of the last decades as a fixed reference. Furthermore, it was acknowledged that the modelling of soil acidify and nutrient availability are the weakest point of the current modelling status.

Although several models are available to simulate dynamics in soil nutrients and pH, here we only focus on the models used by KWR within the WWN, i.e. CENTURY and SWAP-ORCHESTRA, and the WEnR model VSD+ used together with the plant species model Props (Reinds *et al.*, 2015). The idea is that we use the best of these two groups of models to identity the most suitable methods and/or formulations to incorporate into the WWN.

In this report we will first define (in Chapter 2) what is meant by: (i) nutrient availability and (ii) soil acidity in the context of WWN. This is followed by an inventory and comparison of used modelling concepts among the two model systems in view of nutrient availability and acidity. We finalized Chapter 2 with an inventory of strong and weak points of both models. Furthermore an inventory of available relevant datasets that can be used for parametrization and validation is performed (Chapter 3). In Chapter 4 the results are discussed. We conclude this report with conclusions (Chapter 5).

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- STOWA
- Delta program Zoetwater (Ministry of Infrastructure and the Environment)
- Ministry of Economic Affairs
- PNL Netherlands Environmental Assesment Agency
- Provinces of Gelderland, Utrecht and Noord-Brabant
- Water board Aa & Maas and Water board Vechtstromen
- Knowledge program Lumbricus
- Nature conservation organisations Natuurmonumenten and Staatsbosbeheer
- Research Institutes KWR and WEnR

# 2 Model comparison

## 2.1 Assumptions and requirements WWN

Nutrient availability and soil acidity can be interpreted and estimated in different ways. To avoid ambiguity, it is necessary to make definitions of nutrient availability and soil acidity in the context of WWN. Furthermore, we clarify the scope of WWN in terms of their target ecosystems and scenarios to be studied. Clarifying the scope helps to identify which aspects/processes/resolution of nutrient availability and soil acidity need to be considered for successful application of WWN, and therewith to make an effective comparison between different models to predict nutrient availability and soil acidity.

### 2.1.1 Definition of nutrient availability and soil acidity in the context of WWN

The WWN predicts the occurrence probability of vegetation types from nutrient availability and soil acidity via plot-mean indicator values of Witte et al. (2007) for nutrient and acidity (Nm and Rm, respectively) using the framework of PROBE model. Therefore, in the context of WWN, the nutrient availability and soil acidity should be the measures which directly link to the plot-mean indicator values.

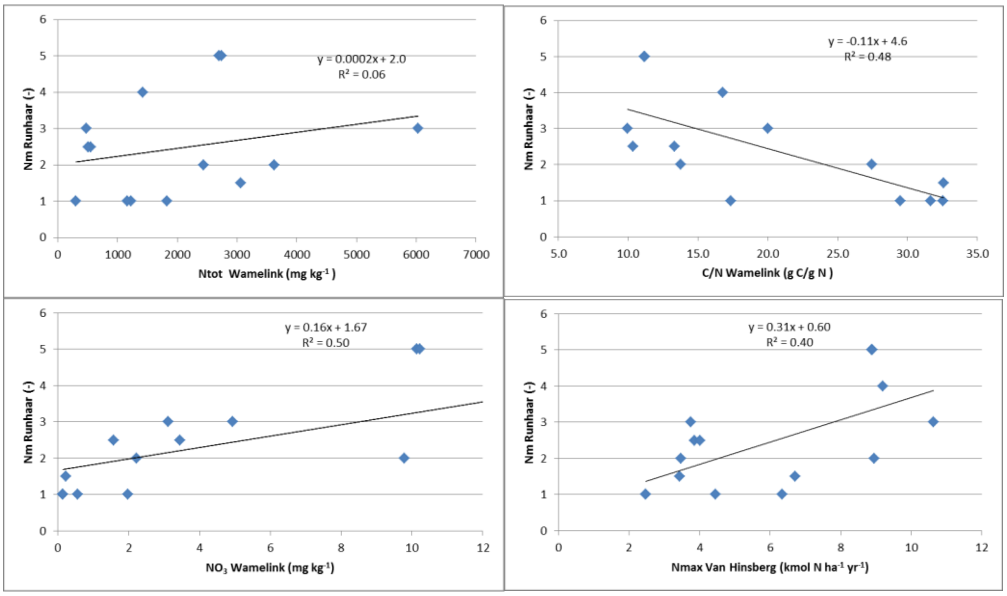
Indicator values of Witte et al. (2007) have been derived from the division of plant species into ecological groups by Runhaar *et al.* (2004). These Runhaar values reflect the vegetation characteristics in relation to environmental conditions, namely salinity, soil moisture, nutrient availability, and acidity. They closely resemble the internationally accepted indicator values of Ellenberg, but are tailor made to Dutch vegetation. Indicator values of a species are determined primarily based on expert judgement on the ‘ecological group’s where the species typically occur. Each ecological group is characterized with ordinal scales of nutrient availability (or ‘potential plant production based on nutrient availability’, divided in: poor/moderate/rich/very rich) and acidity (acid/weakly acid/alkaline). The nutrient availability can also be rephrased as the amount of nutrient available in soil under a given set of abiotic conditions, even if the nutrients cannot be all taken up by plants to produce biomass due to other limitation on plant growth (such as soil moisture, acidity, or development stage). For example, a low-productive pioneer vegetation can still be evaluated as ‘rich in nutrient availability’ if it is judged to contain large amount of nutrients in plant-available forms. Since many species have been ascribed to two or more ecological groups, the ecological amplitude of species are taken into account in calculation of indicator values (see Witte et al. 2007 for details of the calculation). With that, the indicator value describes the preference of each plant species on a continuous scale for nutrient availability (N, ranging from 1.0 = nutrient poor to 3.0 = very nutrient rich) and acidity (R, ranging from 1.0 = acid to 3.0 = alkaline). Next, indicator values of a plot (Nm and Rm) are calculated as an arithmetic mean of the indicator values of all species occurring in the plot. In PROBE, vascular plants and mosses are included for the calculation of plot-mean indicator values.

Existing studies showed that Rm is related to measured soil pH reasonably well (Douma *et al.*, 2012; Cirkel *et al.*, 2014b). However, Rm is less dependent on soil acidity on high pH level, as reflected in the break point ($pH_{KCl}$=5.05) of the regression model of Cirkel et al. (2014b). A similar trend was observed by Schaffers and Sykora (2000), who found that Ellenberg acidity value increases with soil $pH_{CaCl2}$ only until pH 4.75, above which it hardly changes. Cirkel *et al.* (2014b) also found that the explained variance of the relationship between $pH_{KCl}$ and Rm decreased with decreasing groundwater depth. This is because in wet soils plants with aerenchym are capable of releasing oxygen into the soil. By doing so, they can create large pH gradients around their roots, especially in case of upwelling alkaline groundwater.

For this study, we define soil acidity as soil pH (pH_H2O) in the root zone of plants. Since temporal variation of soil pH can be large, even within a growing season (Cirkel *et al.*, 2014b), we suggest to consider either the yearly average or preferably the growing season averaged soil pH. In those cases when pH measurements are available as pH_KCl or pH_CaCl2 we use available robust relationships to transfer those measurements to pH_H2O values (e.g. Fotyma *et al.*, 1998; for pH_CaCl2; Wamelink *et al.*, 2005; for pH_KCl).

Nm is moderately and consistently related to measured nutrient availability (Douma *et al.*, 2012; Fujita *et al.*, 2013; Witte *et al.*, 2015). However, there are a number of measures to express nutrient availability for plants, and the strength of correlation with plant characteristics differs among these measures (Ordonez *et al.*, 2010; Fujita *et al.*, 2013). It was indicated that soil P measures (e.g. P mineralization rate, soil P:C ratio, soil dissolved P) were slightly better related to Nm than soil N measures (e.g. N mineralization rate, soil N:C ratio, soil dissolved N) (Fujita *et al.*, 2013). Furthermore, phosphorus (P) limitation and nitrogen limitation are both common in grasslands of north-western Europa (Van Dobben *et al.*, 2016). Therefore, for this study, we take both N and P into account as two pivotal elements for plant growth. For several habitat types a comparison was made between the optimal Nm Runhaar indicator values and various other corresponding values either based on model results (Van Hinsberg & Kros, 1999), or measurements (Wamelink *et al.*, 2011).

FIGURE 2 COMPARISON OF THE PLOT-MEAN INDICATOR VALUE FOR NUTRIENTS RICHNES (NM RUNHAAR) AND VARIOUS SOIL N MEASURES FOR 15 DUTCH HABITAT TYPES AFTER VAN HINSBERG AND KROS (1999) AND WAMELINK *ET AL.* (2011). THE EXAMINED SOIL N MEASURES ARE MEASURED SOIL TOTAL N (IN MG N/KG; UPPER LEFT), MEASURED SOIL C/N (UPPER RIGHT), MEASURED TOP SOIL NITRATE CONCENTRATIONS (IN MG NO3/KG MEASURED AS EXTRACTABLE IN 1M KCL; LOWER LEFT) (USING THE 75-PERCENTILE), AND MODELED N AVAILABILITY IN TOP SOIL (I.E. SUM OF N MINERALIZATION AND N DEPOSTION; IN KG N/HA/YR, LOWER RIGHT). EACH POINT REPRESENTS A HABITAT TYPE (I.E. AVERAGE VALUES OF SEVERAL PLOTS WHICH FALLS INTO THAT HABITAT TYPE). NOTE THAT NM RUNHAAR IS SIMILAR BUT NOT IDENTICAL TO THE INDICATOR VALUE NM WHICH WE USE FOR THIS STUDY.



We assumed, mineralization rate of N (or P) should better represent nutrient availability for plants than total N (or P), C:N (or C:P) ratio, or extractable N (or P), as it integrates both the nutrient pool and the controlling factors of nutrient turnover (such as temperature and moisture). In fact, mineralization rates were related to Nm slightly better than other measures of N and P at individual stand level (Fujita *et al.*, 2013). The similar trends were observed on an association level (Van Hinsberg & Kros, 1999; Wamelink *et al.*, 2011). It was indicated that modelled levels of N availability, which was sum of N mineralization and N deposition, was better related to indicator value of nutrient richness than soil total N, yet not better than nitrate concentration and C:N ratio (Figure 2). Therefore, we suggest to consider net N mineralization rate (i.e. gross N mineralization minus N immobilization by microbes) as the main source of available N for plants.

N mineralization rates fluctuate largely within and between years. However, Fujita *et al.* (2013) found that time scale with which N mineralization rates were evaluated (i.e, one growing season, one year, or five years) had only minor effect on the relationship between N mineralization and Nm. Therefore, to start with, we choose a time scale of one year to evaluate N mineralization rates as the explanatory variable to predict Nm. See Discussion 4.4 for potential issues of the time scale to be tackled in the Phase 2.

In addition to the mineralization, we also take several other sources of N into account for our estimate of plant available N. In the Netherlands, atmospheric N deposition contributes to a substantial part of mineral N pool in soil. Also, non-symbiotic N fixation (i.e. N fixation by free-living microorganisms) can contribute to a large proportion of mineral N input in low productive ecosystems (e.g. ranging from 0.1 to 21 kg/ha/year in temperate unfertilized grasslands; Reed et al. 2011). Furthermore, in wet systems, N loss via denitrification is not ignorable. Based on these assumptions, we define N availability for plants (Navail, gN/m2/year) as concentration of N-NH4 and N-NO3 in root zone of plants for a period of 1 year, which is formulated as:

Navail = net N mineralization + atmospheric N deposition + asymbiotic fixation – denitrification (1)

We assumed, mineralization rate of N (or P) should better represent nutrient availability for plants than total N (or P), C:N (or C:P) ratio, or extractable N (or P), as it integrates both the nutrient pool and the controlling factors of nutrient turnover (such as temperature and moisture). In fact, mineralization rates were related to Nm slightly better than other measures of N and P (Fujita *et al.*, 2013). Therefore, we suggest to consider net N mineralization rate (i.e. gross N mineralization minus N immobilization by microbes) as the main source of available N for plants. Since timescale of the mineralization estimate had only minor effect on the relationship with Nm (Fujita *et al.*, 2013), we suggest a time scale of one year. In addition to the mineralization, we also take several other sources of N into account for our estimate of plant available N. In the Netherlands, atmospheric N deposition In addition, we consider P inflow via atmospheric deposition and sorption and/or weathering. In short, our definition of P availability (Pavail, gP/m2/year) for this study is:

Pavail = net P mineralization + atmospheric P deposition + P sorption + P weathering (2)

### 2.1.2 Scope of WWN application

The target system of WWN is (semi-)-natural terrestrial ecosystems. It includes different vegetation types (grasslands, forests, heath), different moisture regimes (dry, moist, wet, but not constantly inundated systems such as peat) and different soil types (e.g., sandy, silty, and clayey soils). Former agricultural lands may also be considered. Ecosystems under the influence of brackish water are out of our scope. The WWN is intend to be applicable at the national scale and user friendly so that it can easily be used by the Water Boards,

WWN will be used to evaluate the changes in vegetation due to the results of climate change and water management (which impacts groundwater depths and groundwater level fluctuations). This implies that the chosen models of WWN should include relevant processes of nutrient availability and acidity that are affected by climate change and water management. However, vegetation development is also affected by other environmental influences, like different levels of atmospheric N deposition, vegetation management such as mowing and thinning (and optionally, grazing and sod-cutting too, although these are more complicated to model), and landuse change (e.g. from agricultural lands to nature area). To anticipate on possible future developments of the WWN, the chosen models of nutrient availability and soil acidity should be easily expandable to these environmental influences.

In this following section, we will describe the models which compute the two site factors (nutrient availability and soil acidity), as well as the functional relationships between abiotic factors and the influenced processes for both site factors, e.g. mineralisation, (de)nitrification.

## 2.2 PROBE (SWAP-CENTURY-ORCHESTRA)

### 2.2.1 General description

PROBE is the eco-hydrological model to predict the occurrence probability of vegetation types, developed by KWR and drinking water companies. Modelled habitat factors (soil moisture, soil nutrient availability, soil acidity) are used to predict the response on potential occurrence of vegetation types and the conservation value they represent. The way how the habitat factors are computed is different between versions (Table 1). In PROBE-2.1 (Witte *et al.*, 2015), habitat factors were computed using transfer functions (to speed-up the calculations) derived from mechanistic models such as the hydrology model SWAP (for soil moisture) and the soil module of CENTURY model (for nutrient availability). In PROBE-2.2 (Cirkel *et al.*, 2016a), soil pH was dynamically simulated using the chemistry model ORCHESTRA coupled with SWAP, although the model is not yet fully operational. In PROBE-3 (Fujita *et al.*, 2016), the hydrology model SWAP, soil module of CENTURY, and plant module of CENTURY are dynamically coupled to compute soil moisture and nutrient availability. Due to the dynamic coupling, feedback effects between soil, vegetation, and water are explicitly included in PROBE-3. The soil module of CENTURY includes C, N, and P dynamics. In PROBE-3, pH is not dynamically modelled, but roughly approximated using empirical relationships from Aggenbach *et al.* (2013a) and Stuyfzand (2010).

The primary target system of PROBE is (semi-)natural herbaceous ecosystems. It can be applied for dry to wet ecosystems, but not (yet) for peatlands and for saline ecosystems. The model will be applied and validated for heath ecosystems in an on-going project (BTO 400554/187). PROBE-2.1 was successfully applied to case studies of the catchments ‘Baakse Beek’ (Witte *et al.*, 2015) and ‘Tungelrooyse Beek’ (Van der Knaap *et al.*, 2015; Van der Knaap *et al.*, submitted). PROBE 3 was also applied for an agricultural crop system (Fujita *et al.*, 2016). To apply the model for national-scale prediction of vegetation, we have developed a number of repro-functions and initialization values for different soil types in the Netherlands.

PROBE-2.1 has a user-friendly interface which is the starting point of the WWN. Via the interface, users can select different scenarios of future climate and hydrology. PROBE-2.1 uses geographical input stored as raster maps, enabling prediction of vegetation on a landscape level. The model outputs of PROBE-2.1 are given as maps as well, which show occurrence probability of different vegetation types under different climate scenario as well as conservation values of each cell. Thanks to the use of transfer functions, the computation time of PROBE-2.1 is fast (e.g. three minutes for a catchment area of ca. 270 $km^2$ on a 25 m resolution). PROBE-3 is equipped with a simple user interface and meant for simulation of a single point.

In this report, we primarily present PROBE-3 (for process-based modelling of hydrology, soil, and plants) and PROBE-2.2 (for process-based modelling of soil pH). The linkage between the modules is shown in Figure 3. Note that the dynamic coupling of pH with other model components is not yet realized. The N flows of PROBE3 are schematically shown in Figure 4.

Temporal and (vertical) spatial scales used in PROBE-3 (CENTURY-SWAP) and PROBE-2.2 (SWAP-ORCHESTRA) are as follows. Note that these scales can be adjusted by the user, although the sensitivity of the model outputs to these scales has not been tested.

For the SWAP model, we choose soil layers of 1cm depth for 0 – 600 cm. For the ORCHESTRA model, the soil of 500 cm depth was divided into 65 soil layers, with 1 cm interval for the top 10 cm depth, 5 cm interval for 10 – 60 cm depth, and 10 cm interval for 60-500 cm depth. For CENTURY model, we used 3 soil layers, 0-20, 20-310, and 310-595 cm. In CENTURY, soil organic matter dynamics were simulated only in the top soil layer, while transport of mineral N was simulated all through the layers.

Time step of SWAP varies depending on the relevant process. We chose the time step of a day for SWAP output. Time step of ORCHESTRA and CENTURY were set to be one day. The time step of the CENTURY model can be easily adapted to larger scales, e.g. to the original values of one week for the soil and one month for the plant compartment.

TABLE 1. DIFFERENCE BETWEEN VERSIONS OF PROBE MODEL. EACH VERSION WAS SCORED FOR DIFFERENT ASPECTS 1).

| Version | Model validation | Computation time | pH | Feedback between soil, water, vegetation | Details of processes included | User interface |
|---|---|---|---|---|---|---|
| PROBE 2-1 | +++ | +++ | + | + | + | +++ |
| PROBE 2-2 | + | + | +++ | ++ | ++ | |
| PROBE 3 | ++ | + | + | +++ | +++ | + |

1) +++: main focus, ++: partly addressed, +: slightly addressed

FIGURE 3 LINK BETWEEN DIFFERENT MODULES (E.G. PLANT MODULE, SOIL+LITTER MODULE, HYDROLOGY MODULE, PH MODULE).

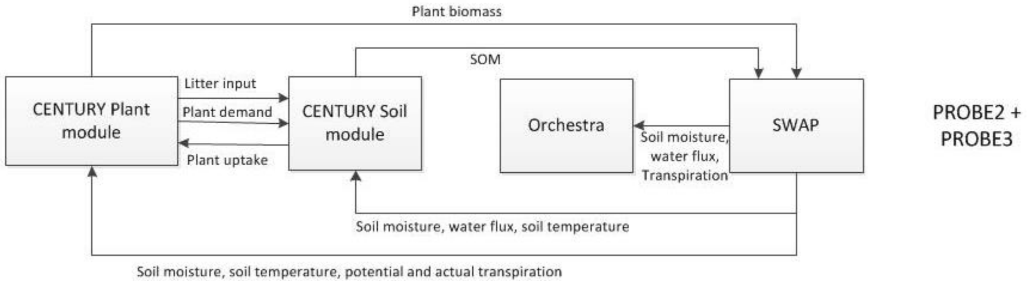
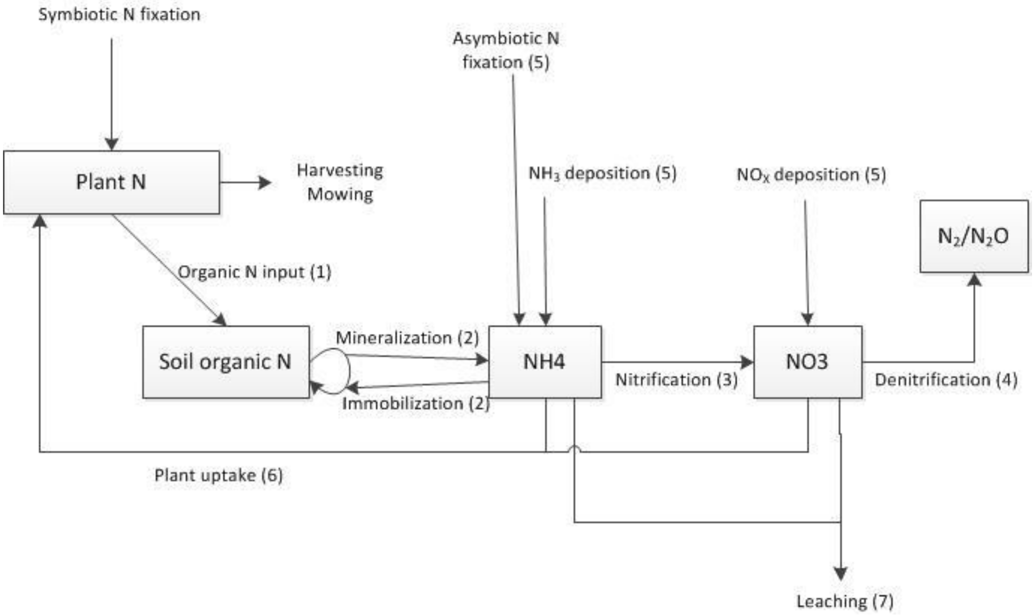


FIGURE 4 SOIL N FLOWS IN CENTURY. NUMBERS IN PARENTHESES INDICATE CALCULATION SEQUENCE.

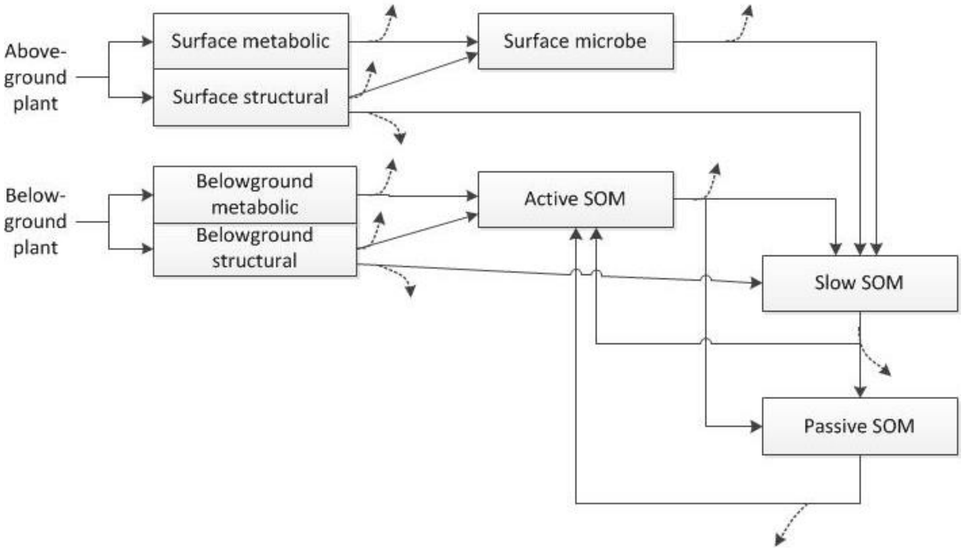


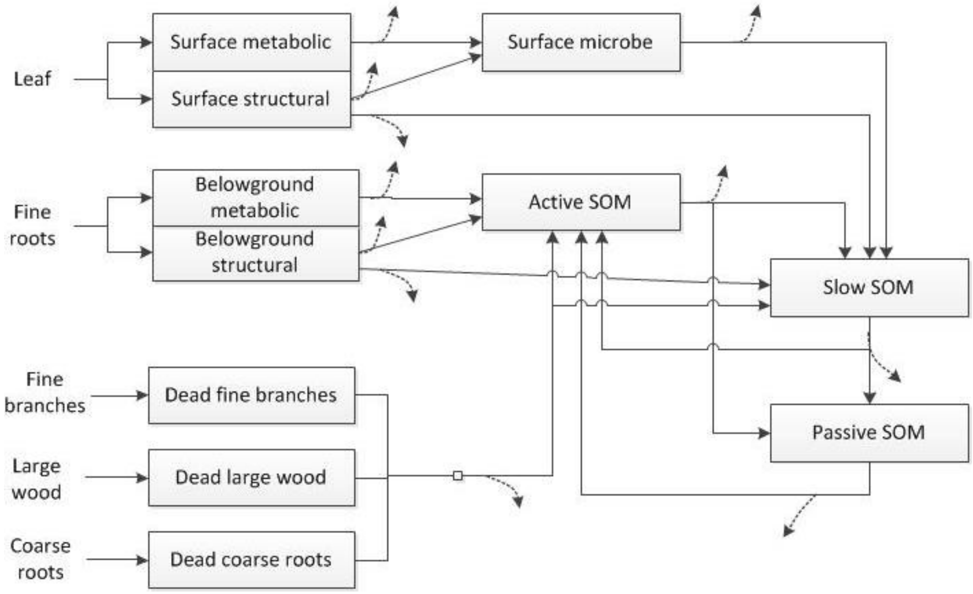
## 2.2.2 Processing

### 2.2.2.1 Decomposition and N mineralization (CENTURY Soil module)

CENTURY includes four carbon pools in soil surface and in soil: three soil organic matter pools (i.e. active, slow, and passive pools), and surface microbial pool. Further, above and belowground plant residues are split into four pools for grasslands (i.e. surface metabolic, surface structural, belowground metabolic, and belowground structural) (Figure 5 above) and seven pools for forests (i.e. in addition, dead fine branches, dead large wood, and dead coarse roots) (Figure 5 below).

FIGURE 5 SOIL ORGANIC MATTER TURNOVERS IN CENTURY FOR GRASSLANDS (ABOVE) AND FOR FORESTS (BELOW). DOTTED LINES ARE THE FLOW OF RESPIRATION (WHICH RELEASES $CO_2$).





Decomposition of carbon is described with simple first-order kinetics as:

$$DEC_i = k_i \cdot C_i \qquad (3)$$

where $DEC_i$ is the amount of decomposed C from pool *i* (gC/m$^2$/day), $k_i$ is the decomposition rate of pool *i* (day$^{-1}$), and $C_i$ is the amount of C in pool *i* (gC/m$^2$).

The decomposition rates are computed by multiplying the pool-specific decomposition coefficient ($kmax_i$, day$^{-1}$) and reduction terms for soil temperature ($rf_{T,i}$) and soil moisture ($rf_{\theta,i}$). Further, the decomposition rate of the active pool is modified by soil texture $rf_{Tex,i}$), and those of surface structural pool and belowground structural pool are modified by lignin content ($rf_{L,i}$).

$$k_i = kmax_i \cdot rf_{\theta,i} \cdot rf_{T,i} \cdot rf_{Tex,i} \cdot rf_{L,i} \tag{4}$$

The decomposition is assumed to be mediated by microbes, with an associated loss of $CO_2$ as a result of microbial respiration. The rate of loss of C by respiration depends on the growth efficiency of microbes. Potential decomposition rate of carbon is thus formulated as:

$$potCmin = \sum_i (1-e_i) \cdot DEC_i \tag{5}$$

where *potCmin* is the carbon mineralized by microbial respiration from all pools (gC/m²/day), $e_i$ is the growth efficiency of microbes when assimilating carbon in pool *i* (fraction between 0 and 1). CENTURY uses constant $e_i$ values except for active pool (i.e. $e_6$), for which increasing clay content linearly increases *e*.

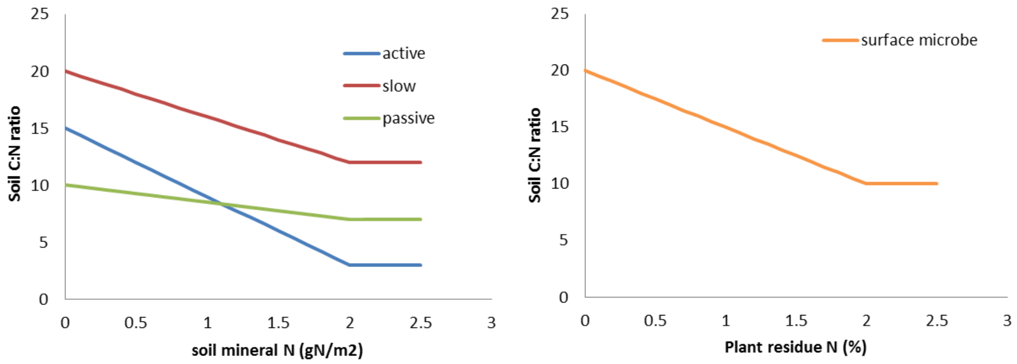
Mineralization and immobilization of nitrogen is strongly coupled with the decomposition of carbon. The N flows follow the C flows and are equal to the product of the carbon flow and the N:C ratio of the pool that receives the carbon. The N associated with carbon loss via respiration is assumed to be mineralized. The amount of N mineralized can thus be formulated as:

$$potNmin_c = \sum_i \sum_j \left( DEC_{i,c} \cdot NC_i - DEC_{i,c} \cdot e_i \cdot NC_j \right) \tag{6}$$

where $NC_i$ is the N:C ratio of the decomposing pool, $NC_j$ is the N:C ratio of the receiving pool.

C:N ratios of structural pools (i.e. surface structural, belowground structural) are fixed as 150, whereas N content of the metabolic pools vary as a function of the N content of the incoming plant residue. C:N ratio of soil microbe and of SOM linearly decreases with increasing amount of N in the incoming plant residues and in soil mineral N pool, respectively (Figure 6).

FIGURE 6 RELATION BETWEEN C:N RATIO AND SOIL MINERAL N (LEFT) AND PLANT RESIDUE N (RIGHT).



When potential N mineralization rate is positive, that amount of N is mineralized and released into the soil mineral N pool. When potential N mineralization rate is negative, that amount of N is immobilized from the mineral N pool. If the N in mineral N pool is not enough to realize the N immobilization, decomposition of carbon is inhibited as follows:

$$I = \begin{cases} 1 & potNmin \geq minN \\ \dfrac{minN}{potNmin} & potNmin < minN \end{cases} \tag{7}$$

where *minN* is the amount of N in mineral N pool (gN/m2), *I* is the inhibition factor (fraction between 0 and 1). Finally, actual rate of carbon and N mineralization are written as:

$$Cmin = I \cdot potCmin$$
$$Nmin = I \cdot potNmin$$

Mineralized N enters the ammonium pool of the top soil.

CENTURY also includes P, it simulates the mineralization of P in CENTURYin the same way as N mineralization.

Decomposed carbon from structural pools, active pool, and slow pool goes to several pools. The flow rates from surface structural pool to surface microbe and slow pools are controlled by lignin content of above-ground plant materials. The flow rates from belowground structural pool to active and slow pools are controlled by lignin content of below-ground plant materials. Flow rates from active pool to slow and passive pools are controlled by soil texture. The flow rates of slow pool to active and passive pools are also controlled by soil texture.

Division of plant residues into metabolic and structural pools are controlled by lignin and nitrogen content in the plant residue.

#### 2.2.2.2 Nitrification and denitrification (CENTURY Soil module)

Nitrification rate follows a first-order process depending on ammonium concentration in soil, and is controlled by soil ammonium concentration, soil moisture, and soil pH.

$$Nit = k_{nit} \cdot [\mathrm{N-NH_4}] \cdot fN_{NH4} \cdot fN_{\theta} \cdot fN_T \cdot fN_{pH} \tag{8}$$

where *Nit* is the nitrification rate (g N/m2/day), *knit* is the maximum nitrification rate (day$^{-1}$), [N-NH$_4$] is the concentration of NH4 in top soil (gN/m$^2$), $fN_{NH4}$ is the reduction term due low concentration of N-NH4 in soil (-), and *fN*θ is the reduction term due to soil moisture (-),fNT is the reduction term due to soil temperature, and $fN_{pH}$ is the reduction term due to soil pH. *knit* is set to be 0.15 day$^{-1}$. Nitrification is limited by moisture stress when soil water-filled pore space is too low and by oxygen availability when water filled pore space is too high. Nitrification is not limited when pH is greater than 7, but decreases exponentially as pH falls below 7.

Denitrification is simulated as a function of concentration of nitrate, CO2 (as a proxy for labile C), and soil moisture:

$$Denit = MIN(fD_{NO3}, fD_{CO2}) \cdot fD_{\theta} \tag{9}$$

where *Denit* is the denitrification rate (g N/m2/day), $fD_{NO3}$ is the denitrification rate limited by NO3 concentration (gN/m2/day), $fD_{CO2}$ is the denitrification rate limited by CO2 concentration (gN/m2/day), and *fD*θ is the reduction factor due to soil moisture (fraction between 0 and 1). Denitrification does not occur below WFPS of 50-60% ; above this threshold it increases exponentially with WFPS. The shape of the slope depends on soil physical characteristics and labile C availability.

#### 2.2.2.3 Inflow and outflow of mineral N (CENTURY Soil module)

Ammonium and nitrate originated from atmospheric N deposition directly enters the ammonium and nitrate pool in the top soil, respectively. Non-symbiotic N fixation is formulated either as a function of precipitation or as a function of N:P ratio in the mineral pool in CENTURY. Since the coefficient values of the non-symbiotic N fixation in CENTURY were obtained by model tuning procedure (Parton et al. 1987) and therefore not underpinned by theoretical or empirical evidence, we use a the median value of Reed et al. (2011), 0.57 gN/m2/yr, as a constant rate of for non-symbiotic N fixation. The fixed N is added to the ammonium pool of mineral N in the top soil layer.

Mineral N is leached from the soil with saturated water flow. CENTURY uses an empirical function to compute the fraction of mineral N which is leached out (as a function of soil texture and monthly saturated water flow). In PROBE, we simulated transfer of dissolved N ($N\text{-}NH_4 + N\text{-}NO_3$) in soil simply as the products of the water flows and the concentration of dissolved N in the originating layer (i.e. advective transport), assuming that dissolved nitrogen and water move at the same advective rate.

#### 2.2.2.4 Plant production (CENTURY Plant module)

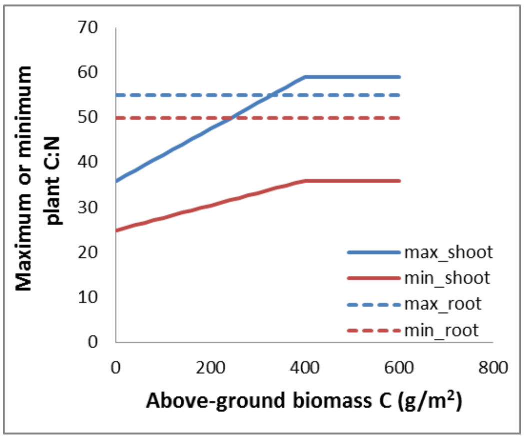
*Plant production in grasslands*

Plant growth of grasslands are simulated dynamically in CENTURY, and are divided into above-ground and below-ground biomass. Potential production of above-ground plant biomass is calculated by plant-specific maximum growth rate, which is modified by reduction terms of soil temperature, soil moisture, and shading effects. The shading effect is calculated as a function of living and dead plant materials, with an assumption that dead plant materials physically obstruct plant production. Potential production of below-ground biomass is computed based on shoot:root ratio. Shoot:root ratio can be either approximated by annual precipitation, or as a function of time since planting. Actual plant production becomes smaller than the potential plant production when currently available N supply (i.e. mineral N available for plants and symbiotic N fixation) is not enough to support the potential production. The fraction of mineral N which is available for plants is computed as a function of root biomass.

N concentration in newly created biomass varies depending on the amount of currently available N supply within the range of pool-specific maximum and minimum C:N ratio, and the maximum and minimum C:N ratio of shoots changes with the size of shoot (Figure 7). Newly created biomass is partitioned into shoot and roots pools, either with a constant rate, or as a function of age.

Decomposition is calculated as a function of soil moisture. In addition, when above-ground plant biomass exceeds a threshold value, plants die at a constant rate. At the senescence month plants die at a constant rate.

FIGURE 7 THE MAXIMUM AND MINIMUM C:N RATIO AS A FUNCTION OF THE SHOOTS BIOMASS.



*Plant production in forests*

The growth of trees is simulated in a similar way to grasses, but their biomass is divided into five components: leaves, fine roots, fine branches, large woods, and coarse roots. Potential production of trees is calculated as potential gross production of trees minus maintenance respiration. The potential gross production is controlled by the effects of soil moisture, temperature, and leaf area index (which is approximated from large wood C pool). The maintenance respiration is calculated as a function of wood N content and temperature. Here it is assumed that only the sapwood part of the tree, which can be approximated by large wood size, respires C. The newly-produced biomass is allocated to different component with specific allocation rates. Leaves die with a month-specific death rate (with options to include the effect of soil moisture, temperature, or day length on leaf death rate). Death rates of other forest components are constant all through the year.

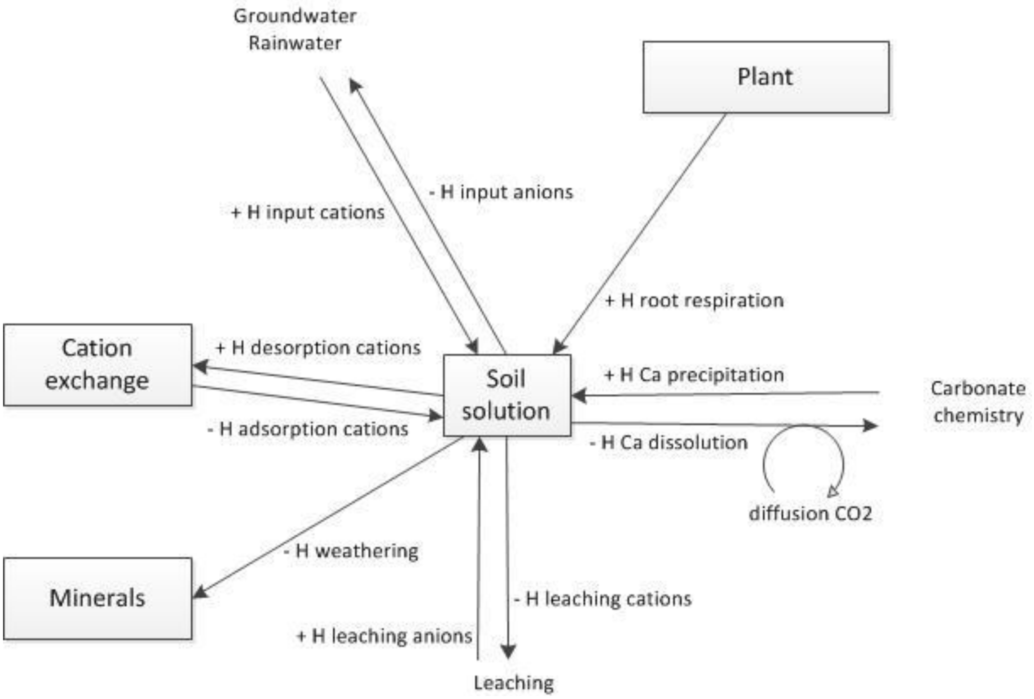
*Plant production in forests with understory*

The growth of forests with understory can be simulated in CENTURY too. It is a combination of growth of trees and growth of grasses, with extra functions to mimic competition between the two groups. Due to competition for light, growth of grasses are suppressed by shading of trees. Competition for nutrient is computed in a way that higher tree basal area and higher amount of mineral N in soil favours the fraction of nutrient uptake by trees.

#### 2.2.2.5 pH (ORCHESTRA)

Soil pH is computed using a set of equations in the program ORCHESTRA (Cirkel *et al.*, 2016a). The model was built primarily for groundwater-dependent grassland systems. Water content and water fluxes between soil layers were simulated with SWAP. Root zone was defined as 40 cm depth. Simulation was conducted with a 1-day time step. In Figure 8 a schematic overview of processes influencing the $H^+$ is given.

FIGURE 8 SOIL $H^+$ FLOWS IN ORCHESTRA.



The geochemical processes included in the model are as follows: adsorption and desorption on organic materials, clay, and oxides; dissolution and precipitation of gibbsite ($Al(OH)_3$) and calcite ($CaCO_3$); pH-dependent silicate weathering; carbonate equilibrium (with $CO_2$ in gas phase); production of $CO_2$ by root respiration as a function of plant production; and gas diffusion of $CO_2$ depending on soil moisture. Uptake of elements by plants is not considered. Time-dependent solute transport (including those from groundwater and rainwater) and gas diffusion (only for CO2) are simulated as well.

In principle, we used the standard parameter values equipped in ORCHESTRA, except following modifications.

Silicate weathering (and contaminant release of $Ca^{2+}$) was modelled with a simplified equation as:

$$W = rw \cdot 10^{0.5 \cdot \left(pH_{ref} - pH_{act}\right)} \tag{10}$$

*W* is the weathering rate ($mol_c/m^2/s/cm$) , *rw* is the maximum weathering rate ($mol_c/m^2/s/cm$), $pH_{ref}$ is the reference pH, $pH_{act}$ is the actual pH. *rw* was set to be $1.15 \cdot 10^{-12}$, $pH_{ref}$ was set to be 3.5.

$CO_2$ production by root respiration was approximated from plant production, which was calculated from transpiration.

#### 2.2.2.6 Hydrology (SWAP)

Soil Water Atmosphere Plant model, SWAP (Van Dam *et al.*, 2008), simulates transport of water in vadoze zones in interaction with vegetation development. SWAP is a one-dimensional, vertically directed model. When the simulated site is groundwater dependent, the daily groundwater level was used as a lower boundary condition. We selected the simple crop module, in which crop-specific and growth-stage-specific parameter values are used to compute upper boundary conditions for soil water movement. For simulation of water loss by evapotranspiration we distinguished between ‘vascular plants’ and ‘bare sand, mosses and lichens’. The potential evapotranspiration of vascular plants was assumed to equal reference crop evapotranspiration according to Makkink (i.e. crop factor of 1.0). Total evapotranspiration was simulated as a cover-weighted average of both groups.

#### 2.2.2.1 Initialisation

CENTURY has a number of approximation rules to aid initialization of state variables and parameter values. For initialization of soil C pools, users need to give values for the soil total C, soil total N, soil total P, and litter C only. The initial amounts of C, N, P in each pool are then computed with vegetation-structure specific fractions to split the total amounts. For vegetation-specific parameters, a set of default values are suggested for each vegetation types.

For multiple-location simulations, we have developed a method to estimate Initial values of soil total C, N, P for CENTURY based on the soil type (‘bodemcode’) of that location (Cirkel *et al.*, 2016a). Similarly, initial values of state variables of ORCHESTRA and initial soil physical characteristics needed for SWAP (e.g. van Genuchten parameters) can be approximated from the soil type.

### 2.2.3 Model outputs

Model outputs of PROBE-3 include values of state variables (on a daily step) such as:

- Organic C and N content in all soil pools and plant components (gC/m$^2$ or gN/m$^2$)
- Mineral N content in all soil layers (gN/m$^2$): nitrate and ammonium separately for the top soil
- Plant biomass of each component (g biomass/m$^2$)
- Soil water content in all soil layers (cm$^3$/cm$^3$)

Furthermore, PROBE-3 also computes daily process rates such as:

- N mineralization/immobilization (gN/m$^2$/day)
- N leaching (gN/m$^2$/day)
- Symbiotic N fixation (gN/m$^2$/day)
- Nitrification and denitrification rates (gN/m$^2$/day)

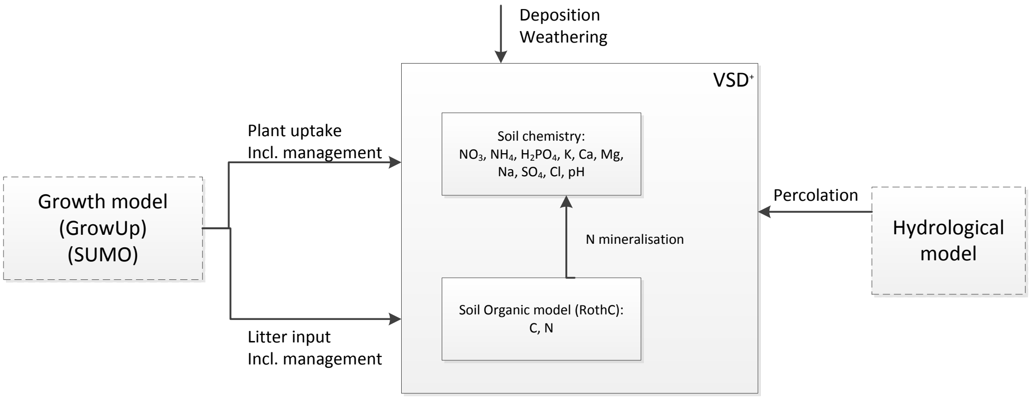
## 2.3 VSD$^+$/GrowUp/SUMO

### 2.3.1 General description

The VSD$^+$ model (Bonten *et al.*, 2016) 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. The VSD+ model is an extension of the VSD model, a very simple dynamic soil acidification model, which has been developed as the simplest extension of steady-state models for critical load calculations and with an eye on regional applications. The model requires only a minimum set of inputs (compared to more detailed models) and execution time is minimised by reducing the set of model equations to a single non-linear equation. To facilitate the exploration of model behaviour at individual sites, the model is linked to a graphical user interface (GUI). This GUI allows easy (Bayesian) calibration, forward simulation (scenario analyses) and can also be used to compute target loads and delay times between deposition reductions and ecosystem recovery. Percolation of water, i.e. water that is leaving the soil compartment, is input and can be obtained by any hydrological model. The same is true for litter input and nutrient uptake by vegetation, which can be obtained by any growth model (Figure 9). The GrowUp application is often used. This is a tool to simulate forest growth, litterfall and nutrient uptake by trees in forest stands, including effects of (simple) forest management. GrowUp allows especially to investigate effects of changes in forest growth and management on VSD+ model (version 1.0 or later) results.

Because the focus in both research and clean air policies has shifted from acidification to the various effects of N deposition and climate change, soil-ecosystem models it includes detailed descriptions of C and N processes, and provide output variables needed for linked vegetation models. The extension in $VSD^+$ consists of descriptions of C and N pools and their interactions, modelled along the formulations of the RothC model (Coleman & Jenkinson, 2014). The $VSD^+$ model can predict both trends and absolute values of (besides $SO_4$, Ca, Mg, K, Na and Cl) $NO_3$ and $NH_4$ concentrations and C/N ratios and pH, which makes the VSD+ model suitable for providing input for plant species diversity models like for instance the vegetation module of PROBE. The C and N model is completely integrated in the VSD+ model. Yearly interactions between pH and decomposition and (de)nitrification take place. The other way around, mineralisation and (de)nitrification affects pH. Litterfall, nutrient uptake and from a hydrological model water percolation and soil moisture are input in VSD+. There is no feed-back between growth and nutrient availability or between growth and water percolation (Figure 9). VSD+ has also been coupled to the succession module SUMO (Wamelink *et al*., 2009), which implies a feed-back between nutrient availability and growth and litter production. With SUMO it is possible to calculated effects of different management options. P is included in the chemical part of the model by Langmuir adsorption and it is part of the charge balance. P is not yet included in the organic part of the model.

FIGURE 9 LINK BETWEEN DIFFERENT MODULES (E.G. PLANT MODULE, SOIL+LITTER MODULE, HYDROLOGY MODULE, PH MODULE). THE VSD+- MODEL INCLUDES A SOIL ORGANIC MATTER PART AND A SOIL CHEMISTRY PART.



SUMO simulates the biomass and nutrient dynamics in the vegetation. The time step of the model is one year. In each time step the biomass, biomass growth, death and removal of biomass are calculated. The growth is in turn calculated on the basis of an assumed maximum growth, which is reduced by nutrient availability (provided by $VSD^+$) and light interception. The dead biomass (litter with nitrogen content) is returned to the relevant pools in $VSD^+$ (Figure 10).

FIGURE 10 LINK BETWEEN DIFFERENT MODULES (E.G. PLANT MODULE SUMO, SOIL+LITTER MODULE, HYDROLOGY MODULE, PH MODULE). THE VSD+- MODEL INCLUDES A SOIL ORGANIC MATTER PART AND A SOIL CHEMISTRY PART.

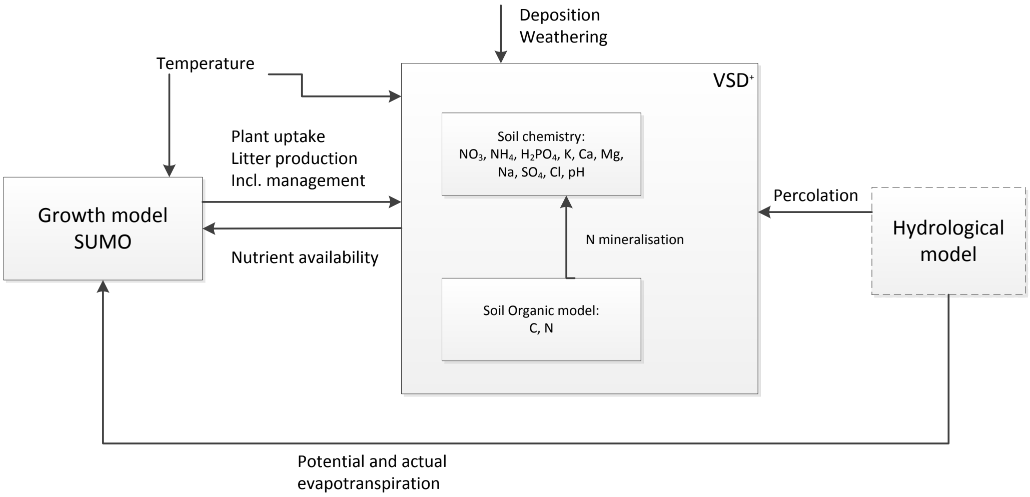
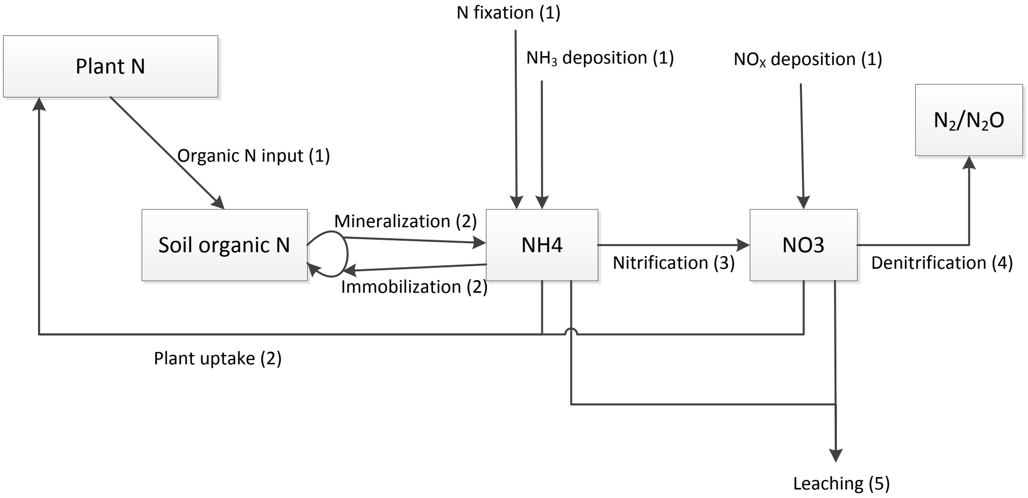


FIGURE 11 SOIL N FLOWS IN VSD$^+$. NUMBERS IN PARENTHESES INDICATE CALCULATION SEQUENCE.

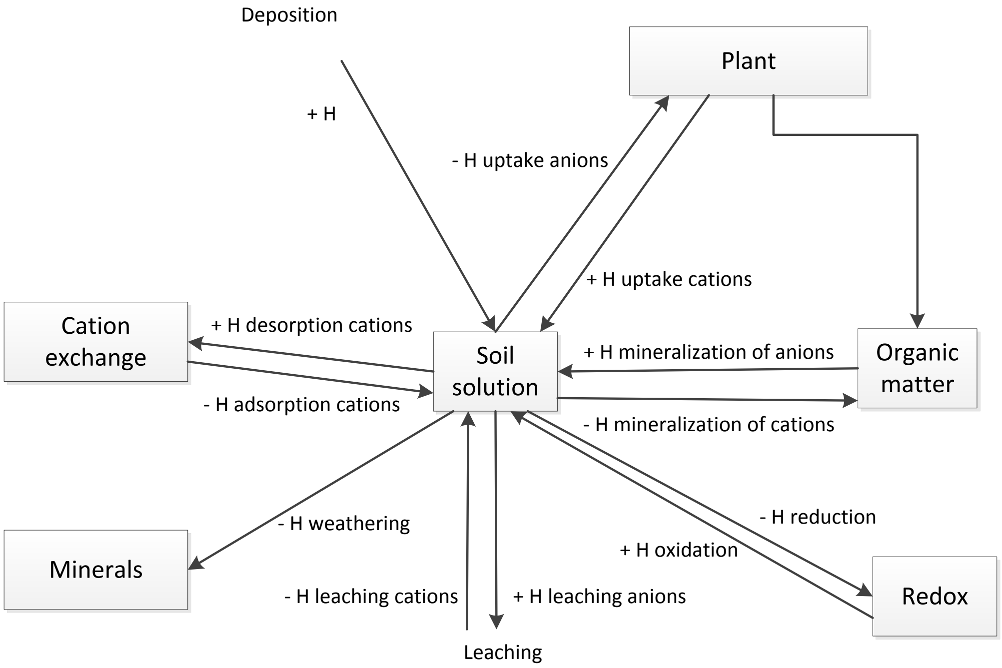


## 2.3.2 Processing

### 2.3.2.1 pH (VSD+)

A schematic overview of processes which influences the flows of H+ is given in Figure 12.

FIGURE 12 SOIL H⁺ FLOWS IN VSD⁺.



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.

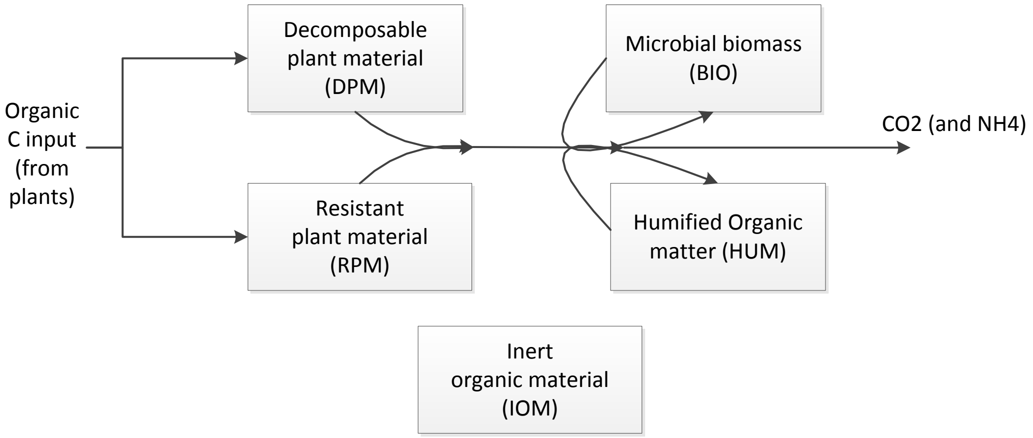
$$\begin{aligned}[H^+] &= [SO_4^{2-}] + [NO_3^-] + [H_2PO_4^-] + [Cl^-] + [HCO_3^-] + [Org^-] \\ &\quad - [Ca^{2+}] - [Mg^{2+}] - [K^+] - [Na^+] - [Al^{3+}] - [NH_4^+]\end{aligned} \tag{11}$$

The changes in the concentrations of elements follow from a mass balance for the individual elements, which describes the change in the total amount of an element over time in the soil. The one side of the mass balance is the total amount of an element, which is the sum of the amounts of the element in the soil solution and in the soil solid phase. 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. 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. The other side of the balance includes the sinks and sources of elements, as well as element leaching as a consequence of water discharge. Sources in VSD⁺ are deposition (all elements), weathering (Ca, Mg, K, Na), input from litterfall (Ca, Mg, K), mineralisation ($NH_4$) and nitrification ($NO_3$). Sinks are leaching, uptake by plants (Ca, Mg, K, $NH_4$, $NO_3$) nitrification ($NH_4$) and denitrification ($NO_3$).

### 2.3.2.2 Decomposition (VSD+)

Decomposition is calculated in VSD⁺ with the formulation of the RothC model (Figure 13).

FIGURE 13 SOIL ORGANIC MATTER TURNOVERS IN VSD+.



Plant material is divided in decomposable and resistant plant material (resp. DPM and RPM), depending on the type of vegetation. The plant material of grass decomposes easier than litter of trees. These two pools decompose to microbial biomass (BIO), humified organic matter (HUM) or to $CO_2$. Also BIO and HUM are decomposing to BIO, HUM and $CO_2$. Each pool, except inert organic matter (IOM), which doesn't decompose, has its own first-order rate constant for turnover and these are modified by temperature, soil moisture and soil cover. The fraction of C turnover from BIO and HUM to $CO_2$ is dependent on clay content.

### 2.3.2.3 N mineralisation (VSD+)

The N fluxes in VSD+ are schematically shown in Figure 11.

The mineralisation and immobilisation of N are dependent on the turnover of the C pools, where the net mineralisation follows from changes in the sum of all organic N pools:

$$N_{mi} = \sum_X \frac{C_{X,yr-1}}{CN_{X,yr-1} \cdot 14} - \sum_X \frac{C_{X,yr}}{CN_{X,yr} \cdot 14} \qquad (12)$$

where $N_{mi}$ (mol m$^{-2}$ yr$^{-1}$) is the N mineralisation; $CN_{X,yr}$ is the C/N ratio of the respective C pool (*X* = *DPM*, *RPM*, *BIO*, *HUM*, *IOM*).

The C/N ratios of RPM, BIO and IOM are fixed, being resp. 100, 8.5 and 10. For DPM the C/N ratio is calculated from the N content of the plant material input. For HUM we assume that with turnover of DPM, RPM and BIO all N in these pools is transferred to the HUM pool.

P mineralisation is not included in VSD$^+$ as SOM in VSD+ only contains C and N. So, mineralisation of base cations is also not included.

### 2.3.2.4 Nitrification and denitrification (VSD+)

Nitrification and denitrification are modelled as first-order processes depending on the total amounts of $NH_4$ and $NO_3$ available after deposition, uptake, mineralisation and nitrification ($NO_3$ only). Inputs for VSD$^+$ are the first-order rate constants and a modifying factor for site-specific climate conditions (in fact temperature and soil moisture). (De)nitrification rates in VSD$^+$ are adjusted for soil pH as follows (De Vries *et al.*, 1988):

$$k_{ni,pH} = k_{ni,ref} \cdot mf_{ni,climate} \cdot \frac{1}{1+\exp(4 \cdot (2.75 - pH))} \qquad (13)$$

$$k_{de,pH} = k_{de,ref} \cdot mf_{de,\mathrm{climate}} \cdot \frac{1}{1+\exp(2.5 \cdot (5-pH))} \tag{14}$$

where $pH$ is the soil solution pH and $k_{ni,pH}$ and $k_{ni,ref}$ (yr$^{-1}$) are the first-order rate constants for nitrification at actual pH and at reference conditions (optimal pH, optimal moisture and $T$ = 10°C) respectively; analogously $k_{de,pH}$ and $k_{de,ref}$ (yr$^{-1}$) for denitrification; $mf_{ni,climate}$ and $mf_{de,climate}$ are the modifying factors for climate conditions for nitrification and denitrification respectively.

### 2.3.2.5 Leaching (VSD+)

Leaching is calculated by multiplying the concentration of the element by the water flux that is leaving the soil compartment.

### 2.3.2.6 N fixation (VSD+)

N-fixation is a given input in the VSD$^+$ model. It is added as done with deposition to the total input of N.

### 2.3.2.7 Forest growth model (GrowUp)

Plant uptake is input in the VSD$^+$ model and is often obtained by the tool GrowUp. Total uptake of N is the sum of growth uptake, which is the net biomass growth times the element contents in the standing biomass, and maintenance uptake, to resupply the losses from litterfall and root decay. N uptake in VSD$^+$ differs from uptake of base cations, for which we use only a net uptake, i.e. growth uptake plus increase in storage in needles for evergreen trees. Implicitly, we thus assume that cations are available immediately after litterfall or root turnover. Uptake of P is incorporated in VSD$^+$ and thus affects the charge balance.

GrowUp is of a module that computes time series of forest growth, nutrient uptake and litterfall, based on data on growth rates forest management in time. Below a short outline is provided of its principles:

Growth and litterfall

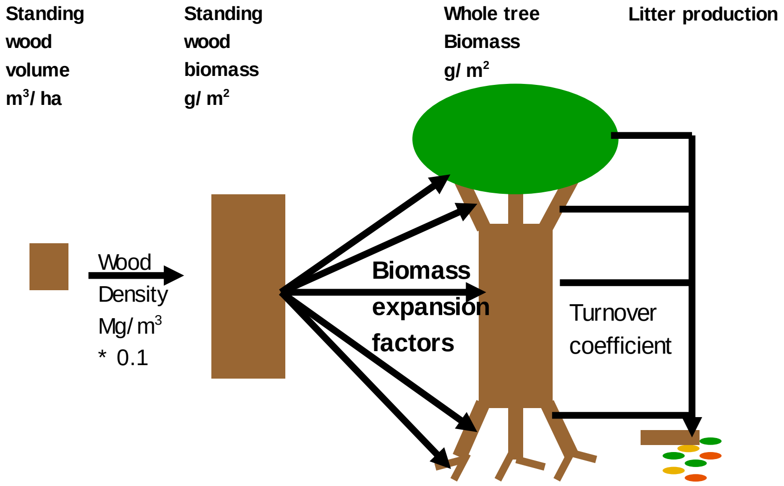
Yearly stem growth is calculated by interpolating the times series of growth rates. Standing biomass of stems is calculated adding yearly stem growth to the standing biomass of the year before. Initial stem biomass is computed as a function of the age of the stand at the start of the run; when the planting date is after the start of the VSD+ simulation, an initial age at the planting year of 2 years is assumed.

Growth of the different compartments (branches, leaves and roots) is calculated according to Equation 1 using yearly interpolated biomass expansion factors (BEFs):

$$Biomass_{compartment} = Biomass_{stems} / BEF_{stems} * BEF_{compartment} \tag{15}$$

The litterfall rates of trees are calculated by functions used in EFISCEN (Schelhaas et al., 2007). The calculation of litter production is visualized in Figure 14.

FIGURE 14 CALCULATION SCHEME FOR THE CALCULATION OF LITTER PRODUCTION



To calculate litter production, we use turnover coefficients per compartment, given as model input parameters, and sum over the compartments (stems, branches, roots, and leaves):

$$Litterproduction = \sum_{Branches}^{Stem} Biomass_{compartment} * Turnovercoeff_{compartment} \tag{16}$$

#### Management

To compute the soil inputs of carbon and nitrogen, information on the forest management is required: e.g. whether whole tree harvesting is practised or stem only and whether root removal takes place at the time of a clearcut. Management actions are limited to planting, thinning and clear cutting. At planting, the biomass starts to grow with an initial age of two years, assuming that two year old seedlings are planted. At thinning or clear cutting, the percentage of removed biomass must be specified and for each compartment (stems, branches, leaves and roots) whether the biomass is removed from the plot or left at the site. When biomass is left at the site, it is added to the amount of litterfall.

#### Nutrient uptake

Nutrient uptake is calculated by multiplying the actual growth per compartment by the contents of nutrients (%) for the compartment. N content in leaves is dependent on deposition according to:

$$ctN_{leaves} = ctN_{leaves,min} + (ctN_{leaves,max} - ctN_{leaves,min}) * (1 - e^{-expNlfdep * Ndep(t)}) \tag{17}$$

Where $ctN_{leaves}$ is N content in leaves (%), $ctN_{leaves,\ min}$ is minimum N content in leaves (%), ctN, max is maximum N content in leaves (%), expNlfdep is the exponent for relation between N in litterfall and N deposition and Ndep(t) is N deposition at time t (eq/m2/yr).

### 2.3.2.8 SUMO

SUMO (Wamelink *et al.*, 2009) distinguishes six vegetation types (grassland, heathland, reedland, shrub vegetation, salt marsh and forest). Each functional type is assumed to consist of three organs: root, stem, and leaf. SUMO calculates biomass growth, death and removal of biomass in view of vegetation management. The model equations are parametrized for each combination of functional plant type and vegetation type. Much attention is given to the simulation of competition between the functional types. The competition for nitrogen The competition for nitrogen and light is assumed to be the driving force for succession. The initial vegetation type is given as input to the model. Apart from biomass growth, SUMO also simulates height growth.

For the functional types herbs/grasses, dwarf shrubs, and shrubs, SUMO simulates the total biomass of all species. For the functional types pioneer tree and climax tree the biomass of a specific tree species is simulated. Each species is given its own set of parameters. The pool of tree species consists of Scots pine (*Pinus sylvestris*), larch (*Larix decidua*), Douglas fir (*Pseudotsuga menziesii*), Norway spruce (*Picea abies*), birch (*Betula pendula* and *Betula pubescens*), ash (*Fraxinus excelsior*), alder (*Alnus glutinosa*), willow (*Salix alba* and *Salix cinerea*), poplar (*Populus* spec.), oak (*Quercus robur* and *Quercus petrea*), northern red oak (*Quercus rubra*) and beech (*Fagus sylvatica*).

SUMO simulates the C and nutrient fluxes (N, P, K, Ca, Mg). The nitrogen that becomes available through mineralization (simulated by VSD$^+$) and atmospheric deposition is partitioned over the functional types and within each functional type over its organs, using fixed percentage distributions per functional type/vegetation type combination. Nitrogen reallocation before litterfall is also simulated.

Biomass

The biomass of each functional type is computed as the result of the biomass in the previous year, the newly formed biomass, the production of dead biomass and the amount of biomass removed by management. The newly formed biomass is the result of the reduction of the maximum growth of each functional type by the reduction factors for light interception and nitrogen availability. Each year, a small amount of biomass is added to each organ of each functional type to simulate seed input (0.0001 ton ha$^{-1}$ y$^{-1}$). For several processes in SUMO the amount of biomass per organ is required. To this end the newly formed biomass is divided over the organs, where the division over the three organs differs per functional type. As with total biomass, the biomass per organ is corrected for death and biomass removal.

Litterfall

Each year part of the biomass dies. The fraction that dies depends on the organ and the functional type, and varies from 1.0 y$^{-1}$ for leaves of herbs, shrubs and deciduous trees to 0.01 y$^{-1}$ for stems of climax trees. The nitrogen content in litter and dead wood is lower than in living material due to reallocation. However, when the nitrogen content drops below a given threshold value no reallocation takes place. The biomass of dead roots and leaves is transferred to the litter pool and nitrogen release from the dead plant parts is simulated by VSD$^+$. VSD$^+$ assumes that dead stems do not release nitrogen.

Nitrogen uptake

The influence of the nitrogen availability on the growth of each functional type is described by a saturation equation based on potential growth, total nitrogen availability, and the minimum nitrogen content per functional type. In principle, all available nitrogen is taken up, but the nitrogen uptake of each functional type is limited by its maximum growth and maximum nitrogen content. The nitrogen that is not taken up by the roots remains in the soil.

#### 2.3.2.9 Hydrology

The hydrology is input to the VSD$^+$ model. Yearly or a constant percolation, i.e. the water that is leaving the soil compartment (m/yr) is needed and a volumetric water content to calculate pools for the mass balance. These values can be obtained by any hydrological model.

### 2.3.3 Initialisation

For the initialisation of soil organic matter content over the five C pools, the inert organic matter pool (IOC) is calculated according:

$$IOC = 0.026.SOC_{ini}^{1.139}.100^{-0.139} \tag{18}$$

where $SOC_{ini}$ is the user provided initial total soil organic carbon content (g $m^{-2}$). Next, the other C pools are initialised by assuming steady state for DPM, RPM and BIO. For DPM and RPM first year inputs are added to the steady state amounts. The C:N ratio of DPM is calculated from the N in incoming plant material ($N_{lf}$) and the C:N ratio of HUM is calculated from the total amount of N in the soil, calculated from the user provided C:N and total soil organic carbon content of the soil, and the C:N ratios of the other C pools.

The initial stem biomass is computed as a function of the user provide stand age.

The initial soil moisture content is calculated by an iterative procedure assuming that the initial amount of soil water equals one-third of the annual precipitation (Bonten *et al.*, 2016).

### 2.3.4 Model outputs

#### 2.3.4.1 GrowUp

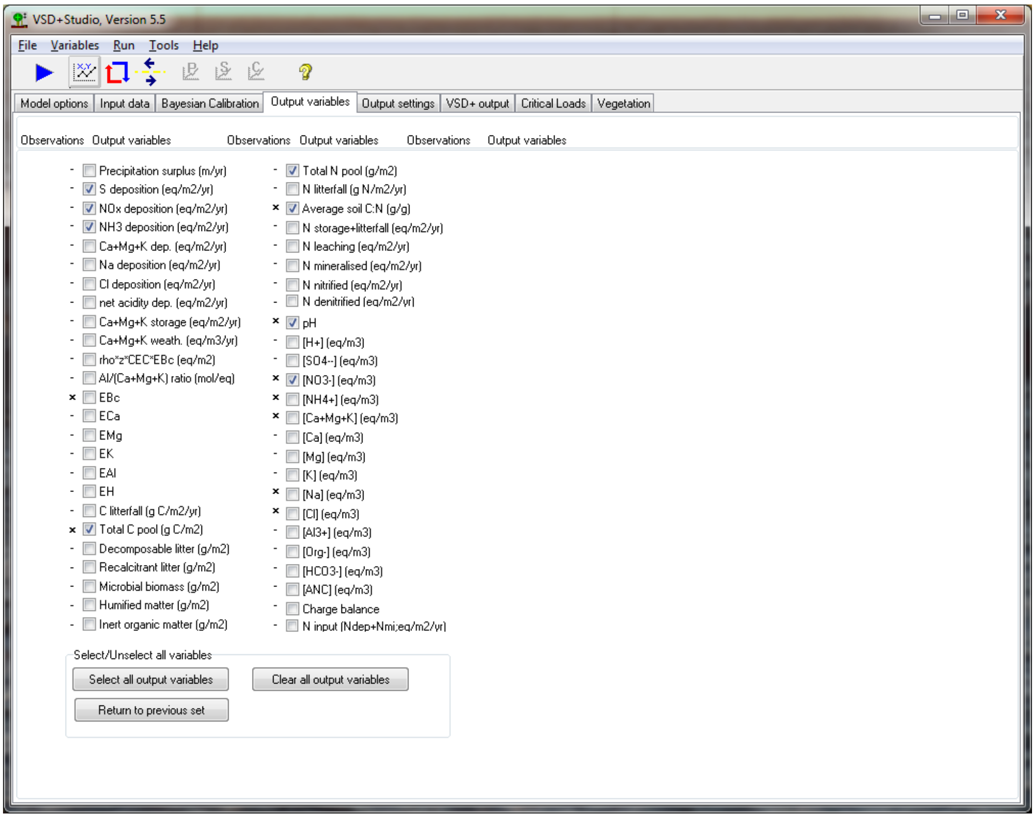
The model output consists of:

- Annual organic C and N input to the soil, which is the total of litter fall, fine root turnover and residues from cutting or thinning (g $m^{-2}$ $yr^{-1}$)
- Annual storage of N, Ca, Mg and K in biomass (e.g. woody biomass on site, or harvested material) (eq $m^{-2}$ $yr^{-1}$)

#### 2.3.4.2 VSD+

Model outputs concern saturation of Ca, Mg, K, Al, and H at the exchange complex, the five organic matter pools, N fluxes like mineralisation, leaching, (de)nitrification and further on the concentrations of all elements in soil solution (Figure 15)

FIGURE 15 SELECTION POSSIBILTIES OF VSD$^{+}$ MODEL OUTPUTS



| Observations | Output variables | Observations | Output variables | Observations | Output variables |
|---|---|---|---|---|---|
| - | ☐ Precipitation surplus (m/yr) | - | ☑ Total N pool (g/m2) | | |
| - | ☑ S deposition (eq/m2/yr) | - | ☐ N litterfall (g N/m2/yr) | | |
| - | ☑ NOx deposition (eq/m2/yr) | × | ☑ Average soil C:N (g/g) | | |
| - | ☑ NH3 deposition (eq/m2/yr) | - | ☐ N storage+litterfall (eq/m2/yr) | | |
| - | ☐ Ca+Mg+K dep. (eq/m2/yr) | - | ☐ N leaching (eq/m2/yr) | | |
| - | ☐ Na deposition (eq/m2/yr) | - | ☐ N mineralised (eq/m2/yr) | | |
| - | ☐ Cl deposition (eq/m2/yr) | - | ☐ N nitrified (eq/m2/yr) | | |
| - | ☐ net acidity dep. (eq/m2/yr) | - | ☐ N denitrified (eq/m2/yr) | | |
| - | ☐ Ca+Mg+K storage (eq/m2/yr) | × | ☑ pH | | |
| - | ☐ Ca+Mg+K weath. (eq/m3/yr) | - | ☐ [H+] (eq/m3) | | |
| - | ☐ rho*z*CEC*EBc (eq/m2) | - | ☐ [SO4--] (eq/m3) | | |
| - | ☐ Al/(Ca+Mg+K) ratio (mol/eq) | × | ☑ [NO3-] (eq/m3) | | |
| × | ☐ EBc | × | ☐ [NH4+] (eq/m3) | | |
| - | ☐ ECa | × | ☐ [Ca+Mg+K] (eq/m3) | | |
| - | ☐ EMg | - | ☐ [Ca] (eq/m3) | | |
| - | ☐ EK | - | ☐ [Mg] (eq/m3) | | |
| - | ☐ EAl | - | ☐ [K] (eq/m3) | | |
| - | ☐ EH | × | ☐ [Na] (eq/m3) | | |
| - | ☐ C litterfall (g C/m2/yr) | × | ☐ [Cl] (eq/m3) | | |
| × | ☑ Total C pool (g C/m2) | - | ☐ [Al3+] (eq/m3) | | |
| - | ☐ Decomposable litter (g/m2) | - | ☐ [Org-] (eq/m3) | | |
| - | ☐ Recalcitrant litter (g/m2) | - | ☐ [HCO3-] (eq/m3) | | |
| - | ☐ Microbial biomass (g/m2) | - | ☐ [ANC] (eq/m3) | | |
| - | ☐ Humified matter (g/m2) | - | ☐ Charge balance | | |
| - | ☐ Inert organic matter (g/m2) | - | ☐ N input (Ndep+Nmi;eq/m2/yr) | | |

## 2.4 Comparison

### 2.4.1 General Overview

Here we present an overview table comparing the principal characteristics of both models (Table 2). An overview of the input data of both models is given in Appendix I.

TABLE 2 OVERVIEW OF THE PRINCIPAL CHARACTERISTICS OF THE PROPE AND SUMU-VSD+ MODELS

| Topic | PROBE (CENTURY-SWAP-ORCHESTRA) 1) | SUMO-VSD$^{+}$ |
|---|---|---|
| Ecosystems | Terrestrial ecosystems, originally developed for agricultural croplands, but now also applicable for natural grasslands, forests, and savannah. Validations both for grasslands and forests. | Terrestrial Ecosystems, like forest, heath and grassland. Most validations on forest. |
| User interface | A simple user interface for a single point application 2) | For single point application easy user friendly interface. For multi-site application the VSD+ dll can be built in in a user program. |
| Computation time | Intermediate (a few minutes for a site for a simulation of ca. 50 years) 3) | Very short, within one minute for the whole of Netherlands (at 250 m by 250 m resolution) |

| Topic | PROBE (CENTURY-SWAP-ORCHESTRA) 1) | SUMO-VSD$^+$ |
|---|---|---|
| Type of input data | CENTURY: 9 field for initial values of state variables of soil<br>11 site-specific parameters (soil)<br>Many fixed parameters<br>Many vegetation-specific parameters<br>SWAP: Daily climate data of 4 variables<br>Ca. 10 site-specific parameters for each soil layer.<br>ORCHESTRA: Many site-specific input data for element concentrations | VSD$^+$: 52 fields with input data and parameters, of which 6 variables need yearly values during the simulation period.<br>GrowUp: 31 fields with input data and parameters<br>SUMO: 8 fields with site specific information. Many fixed parameter values are given in 9 separate input files |
| Time scale | Time steps of one day. Developed for long term effect (e.g. for centuries). | Time step of one year. Developed for long term effects (up to 1000 years) |
| Space scale (horizontal) | Point 4) | Point, but also applied on European scale as an ensemble of multiple points. |
| Spatial scale (vertical) | Three soil layers (with user-specified depth) for the SOM module. Many soil layers (user-specific) for hydrology and pH module. Soil organic matter is simulated only in the top layer. | One soil layer including an organic part and mineral part |
| **Processes** | | |
| Carbon pools | 4 (grassland) or 7 (forest) litter pools:<br>• Surface metabolic*<br>• Surface structural*<br>• Belowground metabolic*<br>• Belowground structural*<br>• Dead fine branches<br>• Dead large wood<br>• Dead coarse roots<br>4 soil pools:<br>• Soil surface microbe<br>• Active pool<br>• Slow pool<br>• Passive pool | 2 litter pools:<br>Decomposable Plant Material (DPM)<br>Resistant Plant Material (RPM)<br>3 soil pools:<br>• Microbial biomass (BIO)<br>• Humified organic matter (HUM)<br>• Inert organic matter (IOM) |
| Decomposition formulation | 1st order, rates are affected by moisture, temperature, soil texture, nutrient limitation, and lignin content | 1st order, rates are affected by moisture and temperature |
| Mineralisation elements | C, N, (P) | C, N<br>Base cations implicit (all are available after litter fall) |
| Nitrification | 1st order, rate affected by temperature, moisture, and pH | 1st order, rate affected by temperature, moisture and pH |
| Denitrification | A slightly deviated 1st order, rate is affected by labile C availability and moisture. | 1st order, rate affected by temperature, moisture and pH |
| Plant uptake | Explicitly calculated. Plant growth is | Model input for VSD+, provided by |

| Topic | PROBE (CENTURY-SWAP-ORCHESTRA) [1] | SUMO-VSD$^+$ |
|---|---|---|
| | affected by temperature, moisture, nutrient availability, and shading. | GrowUp or in feed-back with nutrient availability calculated by SUMO |
| Leaching | Percolation × concentration | Percolation × concentration |
| N fixation | Asymbiotic N fixation: model input<br>Symbiotic N fixation: provides N for plants when mineral N in soil is not enough to support all potential plant growth, with a maximum rate | Model input |
| Exchange | Dzombak-Morel model for hydrous ferric oxide, NICA-Donnan model for Humic acid and Fulvic acid, Donnan model for clay | Gaines-Thomas or Gapon |
| Process order N processes | 1: Organic N input (litter fall)<br>2: Mineralisation/immobilisation<br>3: Nitrification<br>4: Denitrification<br>5: Deposition + asymbiotic fixation<br>6: plant uptake<br>7: Leaching | 1: Deposition + Fixation + organic N input (litter fall)<br>2: Mineralisation/immobilisation + uptake<br>3: Nitrification<br>4: Denitrification<br>5: Leaching |
| Process order pH processes | 1. Net input/output fluxes<br>2. Transport between layers<br>3. Equilibrium calculations, de/adsorption, weathering, $CO_2$ diffusion | 1: Net input fluxes: Deposition, weathering, uptake, (de)nitrification<br>2: Concentrations<br>3: Base saturation and de/adsorption $SO_4$ and $PO_4$ for next year |
| pH effect | Nitrification (Figure 22 left) | Nitrification (Figure 22 left)<br>Denitrification (Figure 22 right) |
| Moisture effect | Plant production (Figure 16 left)<br>Plant death (Figure 16 right)<br>SOM decomposition (Figure 17)<br>Nitrification (Figure 18)<br>Denitrification (Figure 19) | Plant production (only with SUMO) (Figure 16 left)<br>SOM decomposition (Figure 17)<br>Nitrification (Figure 18)<br>Denitrification (Figure 19) |
| Temperature effect | Plant production (Figure 20 top right)<br>SOM decomposition (Figure 20 top left)<br>Nitrification (Figure 20 bottom left) | Plant production (only with SUMO) (Figure 20 top right)<br>SOM decomposition (Figure 20 top left)<br>Nitrification (Figure 20 bottom left)<br>Denitrification (Figure 20 bottom right)) |
| Soil texture effect | SOM decomposition rate (Figure 21 bottom)<br>C flow to slow and passive pool (Figure 21 top left) | C flow to microbial biomass and humus (Figure 21 top right) |

[1] The descriptions of the PROBE model are of PROBE-2.2 (for pH) and of PROBE-3 (for the rest).

[2] PROBE-2.1 is more elaborated, use-friendly interface. This can be adapted for later versions.

[3] PROBE-2.1 has much faster computation time due to their use of transfer functions. This method can be potentially applied for the later versions of the model.

[4] PROBE-2.1 is to be applied for a landscape to national level.

### 2.4.2 Comparison of functional relationships

Below we visualize the difference in functional relationships between abiotic factors and process rates between the two models. See section 2.2.2 and 2.3.2 for details about each process. In section 2.4.3 a brief discussion is given on the included reduction functions.

#### 2.4.2.1 Effect of moisture and temperature

Soil moisture influences plant growth in both CENTURY and VSD+, whereas soil moisture influences plant death only in CENTURY (Figure 16).

Further, soil moisture influences decomposition rate (Figure 17), nitrification rates (Figure 18), and denitrification rates (Figure 19) in both CENTURY and VSD+. The reduction functions are comparable, except that only CENTURY includes reduction effect under wet conditions (Figure 17).

Effects of temperature on decomposition and nitrification rates are similar between CENTURY and VSD+ (Figure 20). Temperature effects on plant growth are similar between the two models in lower temperature range, whereas in higher temperature range only CENTURY has a hampering effect. Temperature effects on denitrification are included only in VSD+.

FIGURE 16 EFFECT OF MOISTURE ON PLANT GROWTH (LEFT) AND PLANT DEATH (RIGHT) IN CENTURY AND SUMO. X-AXIS FOR CENTURY IS ACTUAL TRANSPIRATION DIVIDED BY POTENTIAL TRANSPIRATION, WHICH WERE COMPUTED IN THE HYDROLOGIAL MODULE SWAP. X-AXIS FOR SUMO IS ACTUAL EVAPOTRANSPIRATION DIVIDED BY POTENTIAL EVAPOTRANSPIRATION. SUMO DOES NOT INCLUDE MOISTURE EFFECT ON PLANT DEATH. THE ORIGINAL FUNCTION OF CENTURY WAS ADJUSTED BY FUJITA ET AL. (2015).

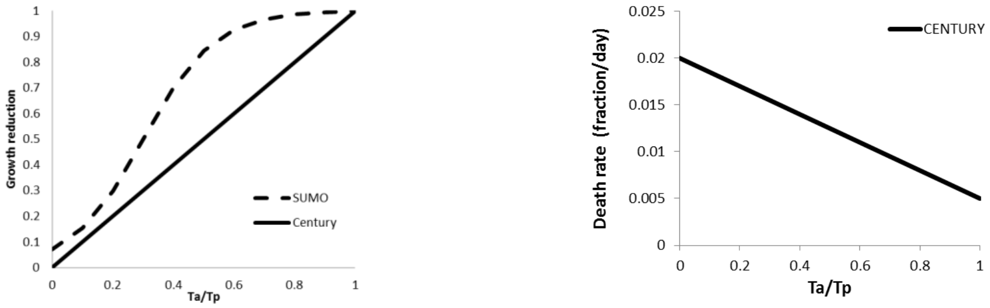


FIGURE 17 EFFECT OF MOISTURE ON DECOMPOSITION IN CENTURY AND VSD+ FOR SAND (‘BOUWSTEEN’ B1, LEFT), CLAY (‘BOUWSTEEN’ B11, MIDDLE) AND PEAT (‘BOUWSTEEN’ B15, RIGHT). X-AXIS IS VOLUMETRIC WATER CONTENT. THE ORIGINAL FUNCTION OF CENTURY WAS ADJUSTED BY FUJITA *ET AL.* (2013) .

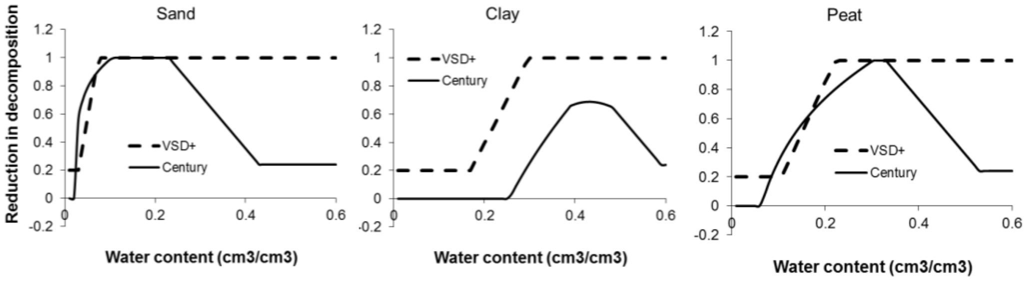


FIGURE 18 EFFECT OF MOISTURE ON NITRIFICATION IN CENTURY AND VSD$^+$ FOR SAND (‘BOUWSTEEN’ B1, LEFT), CLAY (‘BOUWSTEEN’ B11, MIDDLE) AND PEAT ((‘BOUWSTEEN’ B15, RIGHT).

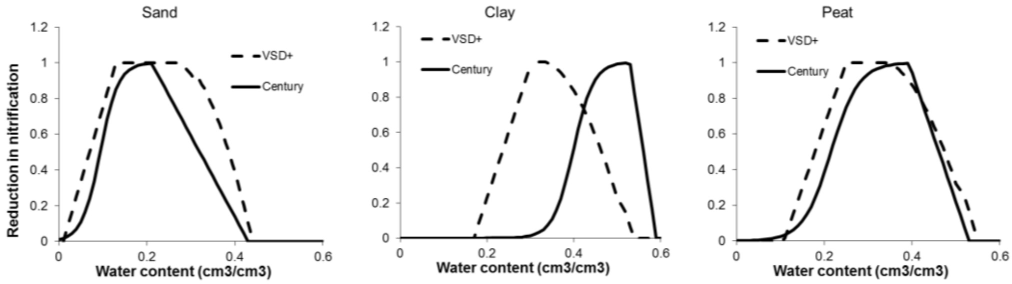


FIGURE 19 EFFECT OF MOISTURE ON DENITRIFICATION IN CENTURY AND VSD+ FOR SAND (‘BOUWSTEEN’ B1, LEFT), CLAY (‘BOUWSTEEN’ B11, MIDDLE) AND PEAT ((‘BOUWSTEEN’ B15, RIGHT).

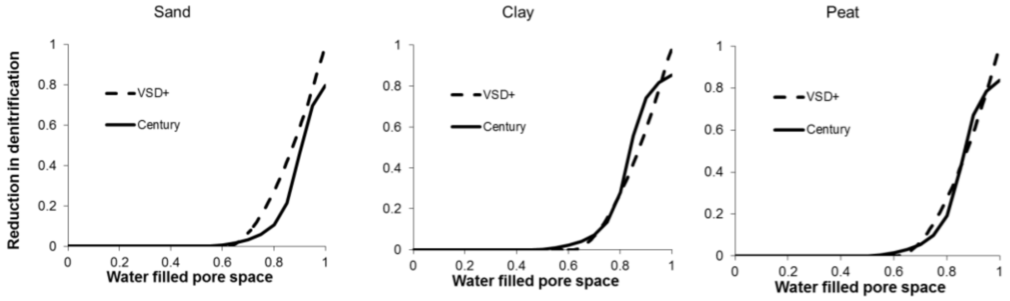
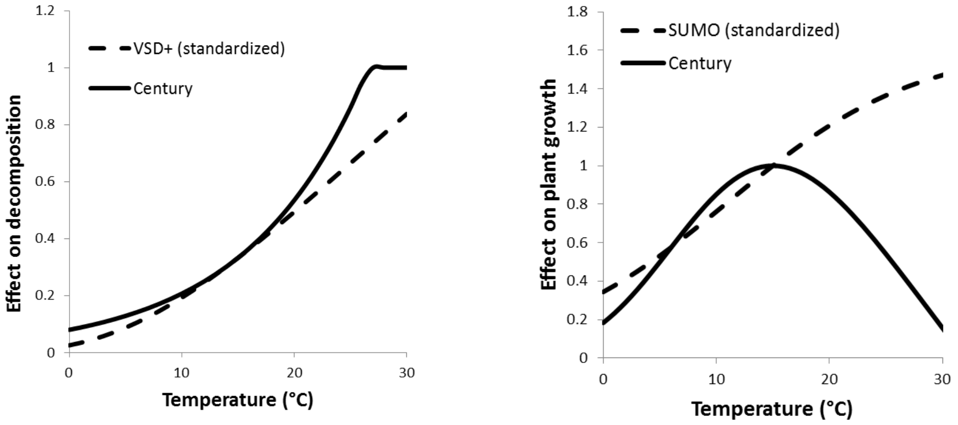
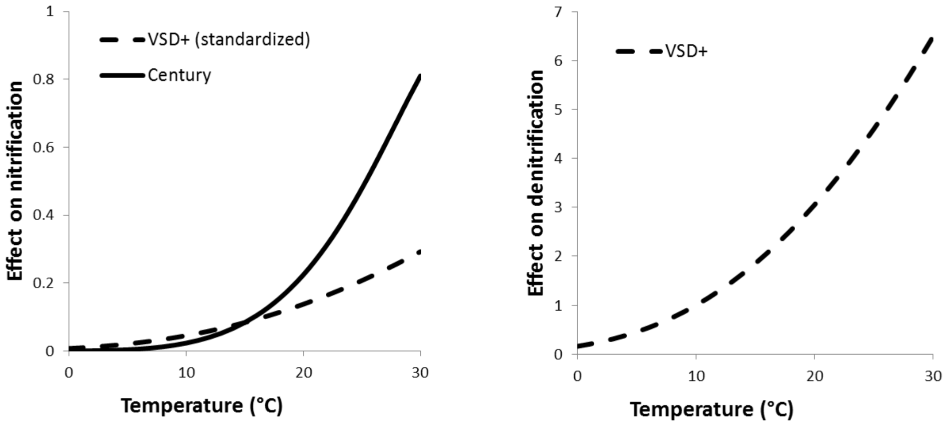


FIGURE 20 EFFECT OF TEMPERATURE ON PLANT GROWTH IN CENTURY AND SUMO (LEFT TOP) AND ON DECOMPOSITION (TOP RIGHT), NITRIFICATION (BOTTOM LEFT), AND DENITRIFICATION (BOTTOM RIGHT) IN CENTURY AND VSD+. FOR THE SAKE OF COMPARISON, THE FUNCTIONS OF SUMO AND VSD+ WERE STANDARDIZED FOR CENTURY AT THE REFERENCE TEMPERATURE OF 15 ˚C. CENTURY USES DAILY AVERAGE SOIL TEMPERATURE OF TOP SOIL (WHICH IS COMPUTED IN HYDROLOGICAL MODULE SWAP), WHILE SUMO AND VSD+ USE YEARLY AVERAGE AIR TEMPERATURE.

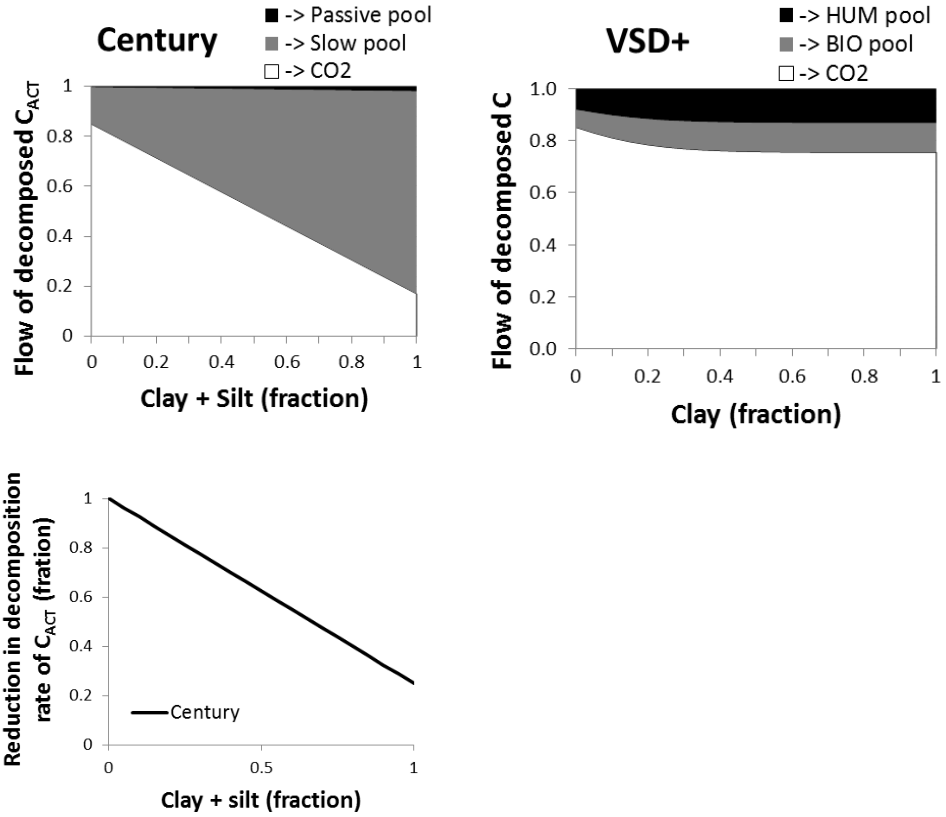




### 2.4.2.2 Effect of soil texture

In both CENTURY and VSD+, a higher clay fraction decreases the fraction of decomposed C that is released as CO2, yet the effect was much stronger in CENTURY (Figure 21 top). Only CENTURY includes the effect of soil texture on decomposition rate (Figure 21 below).

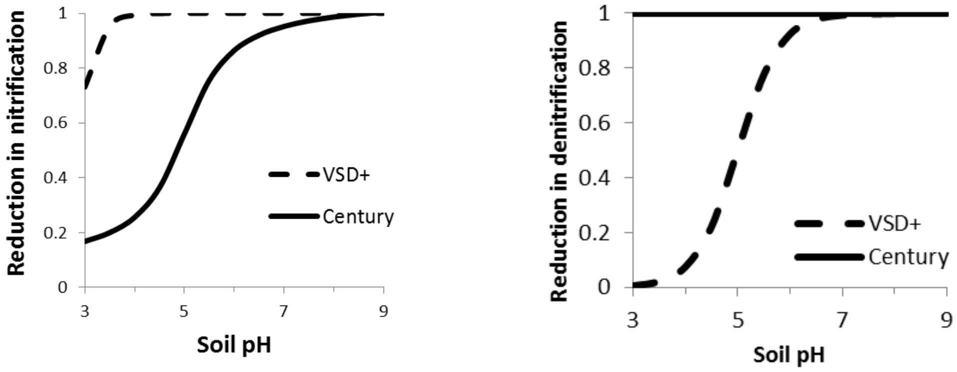
FIGURE 21 EFFECT OF SOIL TEXTURE ON FLOW RATE OF DECOMPOSED CARBON INTO DIFFERENT CARBON POOLS IN CENTURY (TOP LEFT) AND VSD+ (TOP RIGHT), AND ON DECOMPOSITION RATE OF THE ACTIVE CARBON POOL IN CENTURY (BOTTOM).



### 2.4.2.3 Effect of soil pH

Soil pH influences nitrification both in CENTURY and VSD+ (Figure 22 left). The effect of soil pH on denitrification is included only in VSD+ This means that the reduction values is always 1 (Figure 22 right).

FIGURE 22 EFFECT OF PH ON NITRIFICATION IN CENTURY AND VSD+ (LEFT) AND ON DENITRIFICATION IN VSD+ (RIGHT).

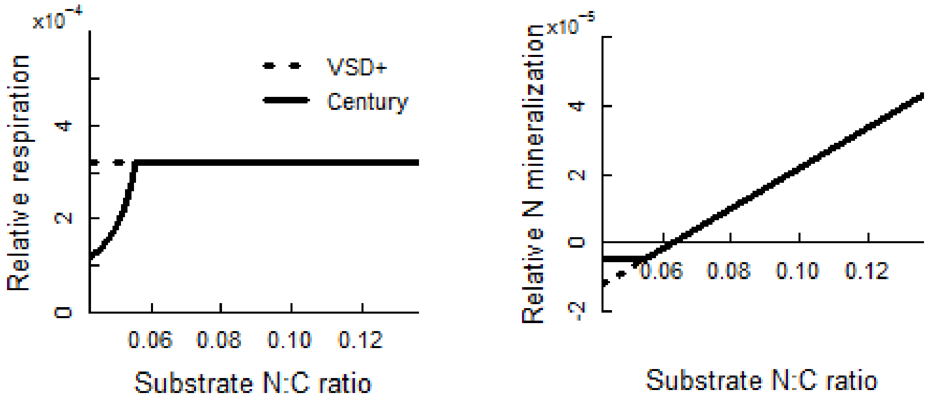


### 2.4.2.4 Effect of soil/litter quality

In VSD+, soil N:C ratio does not influence soil decomposition rate, whereas in CENTURY a low N:C ratio of soil and litter inhibits decomposition (Figure 23 left). Both in VSD+ and in CENTURY, soil and litter N:C ratio influence the amount of N mineralized per unit C decomposed (Figure 23 right), with N-rich substrate releasing more N via mineralization.

Additionally, in CENTURY, lignin content of litter influences decomposition rates and flow rates of decomposed C between pools. In VSD+, so-called ‘litter quality index’, which is a constant parameter value and is different among vegetation types.

FIGURE 23 EFFECT OF SUBSTRATE (I.E. SOIL OR LITTER) N:C RATIO ON RELATIVE DECOMPOSITION RATE (I.E. C DECOMPOSITION RATE PER DAY DIVIDED BY TOTAL C POOL) AND RELATIVE N MINERALISATION RATE (I.E. N MINERALIZATION RATE PER DAY DIVIDED BY TOTAL C POOL) IN CENTURY AND VSD+.



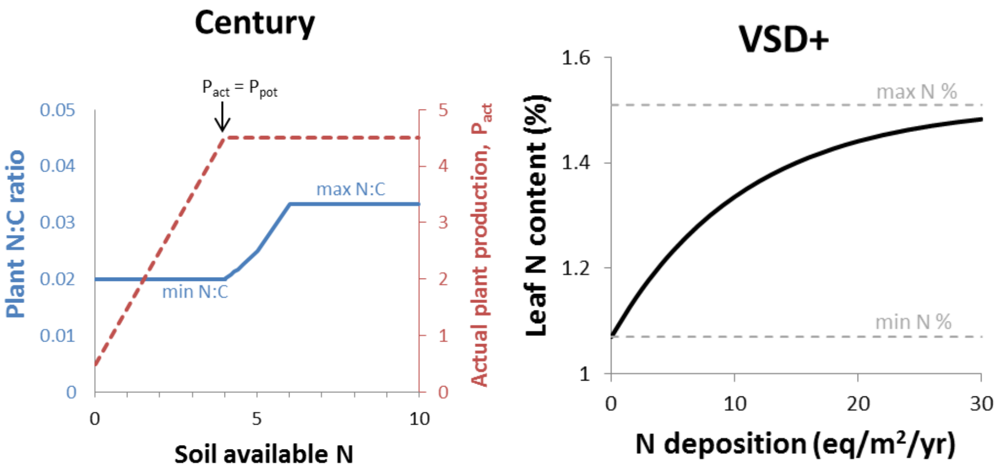
#### 2.4.2.5 Effect of soil N availability/atmospheric N deposition on plant N concentration

Both in CENTURY and VSD+, N concentration in plant changes dynamically, yet with different mechanisms.

In CENTURY, both plant production and plant N concentrations are influenced by soil available N (i.e. N-NO3 and N-NH4). As soil available N increases, actual daily plant production ($P_{act}$) increases up to potential plant production ($P_{pot}$: plant production determined by other factors than nutrients, i.e. moisture, temperature, and shading). After that level, N:C ratio in newly-assimilated plant biomass increases until N:C ratio reaches the maximum value (Figure 24 left). The maximum and minimum N:C ratio is different for shoots and roots, and is a function of size of plant for shoot.

In VSD+, soil available N is not explicitly used to determine N concentration in plants. Instead, annual atmospheric N deposition rate is used to approximate N availability for plants. Similar to CENTURY, leaf N concentration increases as N deposition increases until the vegetation-specific maximum N concentration level (Figure 24 right). An important difference is that plant production is not influenced by N level in VSD+.

FIGURE 24 EFFECT OF N AVAILABILITY ON PLANT N CONC ENTRATIONS IN CENTURY (LEFT) AND VSD+ (RIGHT). MAXIMUM AND MINIMUM VALUES OF N:C RATIO OR N CONCENTRATIONS ARE VEGETATION TYPE SPECIFIC FOR BOTH MODELS. IN CENTURY, ACTUAL PLANT GROWTH ($P_{ACT}$) EQUALS POTENTIAL PLANT GROWTH ($P_{POT}$) AFTER SOIL AVAILABLE N EXCEEDS A CERTAIN LEVEL, ABOVE WHICH PLANT N:C RATIO LINEARLY INCREASES.



### 2.4.3 Discussion on used reduction functions

In addition to the effect on species diversity it is important to consider that the pH influence on soil microbiology cannot be seen independently of the pH influence on plant growth and rhizosphere ecology as they influence the supply and quality of organic matter, i.e. the source of the material to be decomposed (Kemmitt *et al.*, 2006; Pietri & Brookes, 2009). The same is true for temperature and moisture content. E.g. Falkengren-Grerup *et al.* (1998) showed that nitrogen deposition increases the rate of both mineralisation and nitrification.

In general the used reduction functions in both models are quite comparable. Some of the effects are not included in a model but in the other (e.g. temperature effect on plant death, pH effect on denitrification). The difference between models are relatively large in wet conditions and on clay soils. However, these reduction equations can be easily added or replaced without changing model structure. To make a choice on which equation to include in the model, we still need empirical data and knowledge which rationalize the choice.

Notable differences exist for the effect of soil and litter quality and the effects of soil available N. CENTURY takes more process-based approach to reflect these effects. These effects are not easily replaced since it requires changes in model structure (i.e. increases in state variables) or requires different time scale.

### 2.4.4 Comparison of model capacity

We evaluate the possibilities of both models to simulate responses to drivers and factors which are relevant to simulate scenarios on target ecosystems in the context of WWN (Table 3).

TABLE 3 COMPARISON OF VSD+ AND PROBE (CENTURY-SWAP-ORCHESTRA) FOR THEIR CAPACITY TO SIMULATE RESPONSES TO DRIVERS AND FACTORSIN VIEW OF NUTRIENT AVAILABILITY AND PH

| **Responses to drivers/factors for each scenario** | **Relevance for WWN 1)** | | **VSD+** | | **PROBE** | | **Note** |
|---|---|---|---|---|---|---|---|
| | **Nut. availability** | **Soil pH** | **Already included** | **Easy to include** | **Already included** | **Easy to include** | |
| 1.Responses to drivers/factors for each scenario | | | | | | | |
| **Climate change scenarios** | | | | | | | |
| • Temperature effect on SOM decomposition | ++ | | Y | | Y | | |
| • Temperature effect on plant growth / litter production | ++ | | N | Y (using SUMO) | Y | | |
| • Temperature effect on nitrification | - | + | Y | | Y | | |
| • Drought effect on SOM decomposition | ++ | | Y | | Y | | |
| • Drought effect on plant growth / litter production | ++ | | N | Y (using SUMO) | Y | | |
| • Drought effect on plant death | + | | N | Y | Y | | |
| • Drought effect on nitrification | - | | Y | | Y | | |
| • Drought effect on denitrification | + | | Y | | Y | | |
| • Oxygen stress effect on SOM decomposition | ++ | | N | Y 2) | Y | | |
| • Oxygen stress effect on nitrification | - | | Y | | Y | | |
| • Effect of redox status on base and P chemistry | + | ++ | N | N 3) | N | N? 3) | |
| • Effect of short but extreme weather event on SOM decomposition | ? | | N | N 4) | Y | | |
| • Effect of short but extreme weather event on plant death | + | | N | N | Y | | 5) |
| • Effect of short but extreme weather event on groundwater flows | - | ++ | N? | Y | Y | | |

| **Responses to drivers/factors for each scenario** | **Relevance for WWN 1)** | | **VSD+** | | **PROBE** | | **Note** |
|---|---|---|---|---|---|---|---|
| | **Nut. availability** | **Soil pH** | **Already included** | **Easy to include** | **Already included** | **Easy to include** | |
| **Atmospheric N deposition scenarios** | | | | | | | |
| • Effect of N deposition / soil mineral N on plant C:N | ++ | | Y | | Y | | |
| • Effect of N deposition / soil mineral N on plant production | + | | N | Y (using SUMO) | Y | | |
| • Effect of litter and soil C:N on N mineralization rate | + | | Y | | Y | | |
| • Effect of soil mineral N on decomposition rate | + | | N | N 4) | Y | | |
| **Management scenarios** | | | | | | | |
| • Effect of groundwater level on soil moisture | ++ | + | Y | | Y | | |
| • Effect of mowing, thinning, and cleaning on plant biomass | + | | N | Y (using SUMO) | Y | | |
| • Effect of grazing on plant biomass | | | N | N? | N | Y 6) | |
| **2.Responses to factors for specific ecosystems** | | | | | | | |
| **Groundwater-dependent ecosystems** | | | | | | | |
| • Effect of groundwater level on soil moisture | ++ | + | Y | | Y | | |
| • Effect of groundwater recharge on soil water chemistry | | + | N | Y | Y | | |
| **Clay – sandy ecosystems** | | | | | | | |
| • Effect of soil texture on microbial yield efficiency | + | | Y | | Y | | |
| • Effect of soil texture on C partitioning | - | | N | N | Y | | 7) |
| • Effect of soil texture on decomposition rate | + | | N | Y | Y | | |
| **(Low productive) grasslands** | | | | | | | |
| • Effect of nutrient limitation on plant growth | + | | N | Y (using SUMO) | Y | | 8) |
| **Heathlands** | | | | | | | |
| • Competition between trees and grasses | + | | N | Y 9) (using SUMO) | Y | | |

1) Relevance for WWN was evaluated as ++: very relevant, +: relevant, -: indirectly relevant
2) By adjusting the reduction function
3) Lots of extra elements need to be added
4) Smaller time step is needed
5) ‘Oxygen stress ’ module can tackle the effects of extreme event on plant species properly, but not on plant death (and contaminant increase in litter input)
6) Original CENTURY has a set of equations for grazing
7) Otherwise, proper initial partitioning of C pools can tackle this issue
8) Nutrient limitation may also be important in forest ecosystems (but to a lesser extent)
9) Functions of SUMO need to be modified in this regard

### 2.4.5 Strong and weak points

Here we summarize the strong and weak aspects of both model chains in view of modelling soil acidity and nutrient availability.

**PROBE (CENTURY-SWAP-ORCHESTRA)**

*Strong points of PROBE (CENTURY-SWAP-ORCHESTRA) are:*

- Effects of nutrient limitation and C:N:P stoichiometry on plant growth and decomposition are explicitly included
- Dynamic feedback between plant, soil, and hydrology
- Small time step, which enables including temporal aspects, such as seasonality of rain water lenses in areas with upwelling alkaline groundwater, effect of short weather events, and management options
- Explicit inclusion of groundwater influence and carbonate chemistry in pH module

*Weak points of PROBE (CENTURY-SWAP-ORCHESTRA) are:*

- Rather complex with many input (parameter) values
- High computational load
- pH module is not robust for all combinations of input values
- pH module is not coupled with N dynamics in SOM module

**VSD+**

*Strong points of VSD+ are:*

- Relative simple; Relative low data demand
- Includes all macro ions (a complete charge balance)
- Dynamic interaction between pH and biochemical processes.
- With SUMO, it is possible to simulate interactions between soil and vegetation growth and effects of vegetation management like sod cutting and mowing
- Low computational load when applied without SUMO
- Easy to apply (due to link with national database and user friendly user interface)
- Includes P sorption

*Weak points of VSD+ are:*

- C:N ratio of various soil pools constant
- P-mineralisation not yet included
- Combination with SUMO not thoroughly validated
- When combined with SUMO, the number of necessary input values increases a lot
- No seasonal effects due to yearly time step
- No redox

# 3 Available datasets for model parametrization and validation

For the application of the process-based model for a wide range of situations in the Netherlands, we have to assign parameter values to characterise soil- and functional vegetation types. For the parametrization, we need physical and chemical data of soil- and vegetation types.

For the validation of the process-based model we need time series of measured soil processes, contents, concentrations and pools of the main elements.

## 3.1 Datasets for model parametrization

An overview of available dataset for the parametrization is given in Table 4. An extensive overview of the content of each dataset is given in Appendix II. The first 9 datasets are stored in one access database. The dataset 'HUMBASE' (Van Delft, 2001; Van Delft *et al.*, 2012; Van Delft, 2013) includes 1864 soil profiles gathered in heathland and grassland, of which a majority is for agricultural use. A selection of 'nature' sites with chemical analyses (296 sites) was made for KWR. That part is described here. Note that the considered datasets also contain model output, but only during one time. The lack of time series make them unsuitable for model validation.

TABLE 4 OVERVIEW OF POTENTIAL DATASETS FOR PARAMETRIZATION.

| Name/Ref | Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|---|
| (De Vries & Leeters, 2001) | 150 forest sites sampled once in 1990 | Soil, soil solution and vegetation | All major elements and pH |
| (De Vries *et al.*, 1995) | 12 forest sites on non-calcareous soils sampled once in 1992 | Soil, soil solution and vegetation | All major elements and pH |
| (De Vries, 1993) | 48 forest sites on sandy soils (calcareous and non-calcareous) sampled once in 1992 | Soil, soil solution and vegetation | All major elements and pH |
| (Klap *et al.*, 1999b) | 40 forest sites on loess soils sampled once in 1992 | Soil, soil solution and vegetation | All major elements and pH |
| (Klap *et al.*, 1999b) | 30 forest sites on clay soils sampled once in 1992 | Soil, soil solution and vegetation | All major elements and pH |
| (Klap *et al.*, 1999b) | 30 forest sites on peat soils sampled once in 1992 | Soil, soil solution and vegetation | All major elements and pH |
| (Klap *et al.*, 1999a) | 63 grassland and forest sites in the Drentse Aa region sampled in 1994 | Soil, soil solution and vegetation | All major elements and pH |
| (Leeters & de | 200 forest sites on non- | Soil, soil solution and | All major elements and |

| | | | |
|---|---|---|---|
| Vries, 2001) | calcareous soils sampled once in 1995 | vegetation | pH |
| HUMBASE | 296 grassland, heath and forest sampled once in the period 1990 – 2013 | Soil solid phase | All major elements, pH and C and N pools |
| (Fujita *et al*., 2013) | 36 Grasslands, heath, sampled once in 2011 | Soil, vegetation | C, N, P, pH |
| (Ordonez et al. 2010) | 51 grasslands, shrubs, forests, sampled once | Soil, vegetation | C, N, P, pH |
| (Olde Venterink *et al*., 2002) | 47 grasslands | Soil, vegetation | C, N, P, pH |

## 3.2 Datasets for model valdation

inventories at 10 sites with time series that are in principle suitable for model validation as given in Table 5. An extensive overview of the content of those datasets is given in Appendix III.

TABLE 5 OVERVIEW OF POTENTIAL DATASETS FOR VALIDATION.

| **Name/location** | **Data type** | **Vegetation structure** | **Measurements** | **Reference** |
|---|---|---|---|---|
| Speulderbos | monthly or weekly monitoring (1990-1995) | forest | Soil pore water (major elements, pH)<br>Deposition | Van der Salm *et al.* (1998) |
| Risdalheia | Yearly$^{*1}$ monitoring 1984-1997 | forest | Soil pore water (major element)<br>Mineralization<br>Nitrification<br>Litterfall<br>Plant nutrient (N, K, Ca, Mg)<br>Deposition | Mol-Dijkstra and Kros (2001) |
| OBN Sites | Monthly monitoring in 1999, 7 sites | grassland | Soil pore water (major elements) | Grobben et al., (unpublished data)<br>(Kemmers, 1999; Kemmers *et al*., 2000) |
| Veenkampen | Monitoring 1983-2006 | grassland | Soil C & N & P & K pool<br>Soil pore water (major elements)<br>Plant biomass, N & P & K content | Mol et al., (unpublished data) |
| Hulshorsterzand | Chronosequence, measured in 1993-1994 | Bare soil to forest | Soil C & N pool<br>Plant biomass<br>Plant species composition | (Wamelink *et al*., 2001) |
| Sellingen | Chronosequence , measured in 1999 | forest | Soil pore water (major elements)<br>Soil C & N pool<br>Plant biomass & nutrient content | (Wamelink *et al*., 2001) |
| ECN database, UK | 1992-2011, 12 sites (ca. 100 plots) | Grassland, forest | meteo (hourly)<br>deposition (weekly)<br>soil solution chemistry (bi- | |

| | | | | |
|---|---|---|---|---|
| | | | weekly)<br>vegetation surveys | |
| Luchterduinen | Chronosequence, measured in 2012, 110 sites | Bare soil to grassland | Soil C & N pools<br>pH<br>Plant species composition<br>Plant biomass | (Aggenbach *et al.*, 2013b) |
| Hoge Veluwe | Monthly monitoring 3 lysimeter (2016 – 2018) | Heath | Leachates (N-NO3, N-NH4, DON, P-PO4)<br>Meteo<br>Soil pore water (N-NO3, N-NH4, DON, P-PO4)<br>Soil C & N & P pool<br>Plant biomass, N & P content<br>N dry deposition | Fujita et al., unpublished |
| Castricum | Monthly monitoring 4 lysimeters, 1941-1999 | Bare, grassland, forest | Leachates (Major elements)<br>Meteo<br>Deposition | (Stuyfzand & Rambags, 2011)& |

*1: Some of the variables were measured more often than yearly interval.

### 3.2.1 Speulderbos

The Speulderbos was in 1998 a 40 year old Douglas fir stand in the Netherlands (planted). The soil is sandy loam (Boxman *et al.*, 1995; Van der Salm *et al.*, 1998). In 1989, a 2-3 m high transparent roof was erected to intercept throughfall before it reached the forest floor. Part of the roofed area received ambient deposition, whereas the other part received deposition with pristine amounts of N and S. Until 1992 the collected throughfall was sprinkled every two weeks. This system was replaced by an almost real time watering in February 1992. A complete description of the experimental design and the monitoring program is given in Boxman *et al.* (1995). Ceramic lysimeter cups were installed in the mineral soil of each plot at depths of 10 cm (eight replicates), 25 cm (four replicates), 45 cm (four replicates) and 90 cm (four replicates). Boxman *et al.* (1995) only analysed the averaged value of the replicates and paid no attention to the strong spatial variation among the replicates. Van der Salm *et al.* (1998), however, calculated 95% confidence intervals per plot for each observation date from 1990-1994 and found strong fluctuations in soil solution between the individual cups in both the roofed plot with ambient and with pristine deposition. The coefficient of variation ranged between 30 and 150%. Accordingly, the 95% confidence interval around the measurements was rather broad, especially in dry periods when no soil solution could be extracted from some of the cups. Moreover, the lack of soil solution data from these cups, situated in the dryer part of the plot, may lead to an underestimation of the average concentrations during these dry periods.

### 3.2.2 Risdalsheia

Risdalsheia is located near Grimstad, southern Norway, (58°23'N, 8°19'E) at 300 m above sea level (Wright et al., 1998a). The site is representative of large areas of upland southern Norway. Mean annual precipitation is 1400 mm, runoff is 1200 mm and mean annual temperature is 5°C (mean of –3°C in January and +16°C in July). Vegetation is mainly a sparse cover of pine (Pinus sylvestris L.) and birch (Betula pubescens L.) with heather (Calluna vulgaris L.) and blueberry (Vaccinium myrtillus L.) as dominant ground species. Risdalsheia receives relatively high levels of acid deposition with mean values for 1984–1992 of 113 meq S $m^{-2}$ $yr^{-1}$ and 132 meq N $m^{-2}$ $yr^{-1}$ (Wright et al., 1993).

### 3.2.3 OBN, 7 locations on (relatively) wet ecosystems

Seven research plots of OBN at wet grasslands all over the Netherlands were used for a validation of SMART2 (not published). Many soil properties were measured, but soil solution concentrations only for one year.

### 3.2.4 Veenkampen

The Veenkampen is a research site located between Wageningen and Veenendaal. The soil consists of a clayey topsoil on peat. At the beginning of the twentieth CENTURY the vegetation consisted of a species rich grassland vegetation, but after 1945 is the area drained and levelled for agriculture. From 1968 to 1978 was the annual fertilization 300 kg N, 33 kg P and 125 kg K. Since 1978 is the fertilization stopped and mowed twice each year. In 1986, rewetting experiments began and the plot was divided in a dry part, with the same hydrological regime as the surrounding plots, and a wet part. Those two parts were subdivided into different parts with different types of management were applied.

### 3.2.5 Hulshorsterzand

This dataset is based on a chronosequence from bare soil to forest of a nutrient poor ecosystem (Berendse, 1998; C. G. F. De Kovel, unpublished data) located in the Leuvenumse Bos (52˚20’’ N, 5˚44’’ E). The substrate in these areas consists of unconsolidated calcium-poor material of fluvio-glacial origin with a thin cover of aeolian deposits. Vegetation development in such inland dune areas can be considered as primary succession. Within these areas, different parts (sites) have been colonized by vegetation at different times in the past, so that different stages of succession coexist. Since the substrate is homogeneous and spread over large areas, different sites with different stages of succession form a successional chronosequence. Each site, though, has its own history of atmospheric deposition.

### 3.2.6 Sellingen

This dataset is based on a Chronosequence of oak forest on former agricultural land, Eastern Groningen (in the neighbourhood of Sellingen). The oaks were planted as 3-year old seedlings on ploughed soil. The original number of seedlings is unknown. The sites were extensively managed and weed-control or thinnings have not been carried out. At the time of the measurements the stands were 4, 8, 11 and 18 years old (Van der Salm *et al.*, 2006). The stands were located close to the village of Sellingen (52°56″N, 7°05″E) in the northeastern part of The Netherlands. The oaks were planted as 3-year old seedlings on ploughed soil. The original number of seedlings is unknown. The sites were extensively managed and weed-control or thinnings have not been carried out. At the time of the measurements the stands were 4, 8, 11 and 18 years old. The stands were located close to the village of Sellingen (52°56″N, 7°05″E) in the northeastern part of The Netherlands. Rainfall, throughfall, soil water contents, groundwater level and the water level of the ditches was measured once a month from June 2001 to January 2003. Throughfall was measured using 10 samplers at each site. The funnels (18 cm diameter) were placed in a cross in each stand at varying distances to the tree stems. Rainfall is collected in two open fields at approximately 500 m from the sites. Soil water contents were measured at three points in each site using plastic access tubes and a portable TDR probe. Soil solution was sampled using lysimeter cups made of polyester acrylat. Cups were installed at 10, 30 and 90 cm depth. At each depth 15 lysimeter cups were placed at randomly selected sites within each plot

### 3.2.7 ECN database UK

We have obtained data of several plots in the UK. They all have a long complete time series of meteo (hourly), deposition (weekly), soil solution chemistry (bi-weekly) and vegetation surveys (about 100 plots). Table 6 gives an overview of the available time series. A description of the monitoring sites is given In Appendix III. Unfortunately, soil properties are not available in this set.

TABLE 6 TIME SERIES AVAILABLE IN ECN DATABASE.

| Sites | Meteo | Precipitation chemistry | Solution chemistry | Vegetation surveys | |
|---|---|---|---|---|---|
| Alice Holt | 94-11 | 94-11 | 94-09 | 94 | |
| Cairngorms | 99-11 | 99-10 | 99-10 | 98-99 | |
| Drayton | 93-11 | 93-10 | 94-09 | 93 | |
| Glensaugh | 94-11 | 93-10 | 93-10 | 94 | |
| Hillsborough | 93-95,01-09 | 94-09 | 94-10 | 94 | |
| Moor House | 92-11 | 92-11 | 92-11 | 93-94 | |
| North Wyke | 95-11 | 93-10 | 10 | 93-94 | |
| Porton | 92-12 online | 94-10 | 96-99 | 91,94 | |
| Rothamsted | 93-11 | 92-11 | 94-11 | 93 | |
| Snowdon | 95-09 | 97-10 | 97-10 | 95,97-00 | |
| Sourhope | 93-11 | 93-10 | 93-10 | 93-94 | |
| Wytham | 92-11 | 93-12 | 93-10 | 93-94 | |

### 3.2.8 Lysimeters in Hoge Veluwe

KWR installed six precision lysimeters in a heath stand in Hoge Veluwe. From three lysimeters, leachates from 50 cm depth are monthly collected for chemical analysis between December 2016 and spring of 2018. At the same sampling interval, soil pore water of 10 cm, 25 cm, and 50 cm depth are also collected from nearby locations (N=3). In summer 2017, soil bulk properties (C & N & P pool) and plant properties (biomass, N & P content) will be measured. Next to the lysimeters, RIVM measures dry deposition of nitrogen.

### 3.2.9 Luchterduinen

Based on analysis of high-resolution aerophotographs, chronosequence of dune grasslands were built in lime-rich and lime-poor dunes in Luchterduinen. The chronosequence includes different ages of dune grasslands, ranging from 0 to 97 years old. Soil C and N pools, plant biomass (only for a part of the plot), and plant species composition were measured.

### 3.2.10 Lysimeters in Castricum

There exist long-term datasets of four lysimeters in Castricum. The dimension of the lysimeters is 25 x 25 x 2.5m. The vegetation in the lysimeters (at the time of the installation) is: bare sand, shrub, pine forest, and oak forest. Apart from measurements of meteorology and deposition, chemical properties of leachates were measured monthly. Measured items in the leachates are: SEC, pH, Cl, $SO_4$, $HCO_3$, $NO_3$, $NO_2$, $PO_4$, Na, K, Ca, Mg, Fe, Mn, $NH_4$, $SiO_2$, KMnO4, colour (till 1961), NH4-album (till 1961), TOC (after 1980).

# 4 Discussion

In general terms the two model chains are quite comparable. This was also found in other comparative studies. In a an overview paper on the use of dynamic soil–vegetation models to assess impacts of nitrogen deposition on plant species composition, De Vries *et al.* (2010) concluded that there are large similarities between those type of models (not including VSD+ and PROBE), particularly those based on survey data, but there are also several important differences, including: (1) use of different abiotic variables for N, such as N availability (such as VSD+ and PROBE), Ellenberg N indicators and soil-solution N, (2) prediction of individual plant species versus. plant communities, and (3) calibration based on different (national) soil and vegetation data sets.

Nevertheless, there are clear differences exists between two reviewed modelling chains. In sequel of this section we address the following discussion points:

- The background/origin of the discussion point
- The consequences for the model results
- The feasibility of changing/including the discussed item

## 4.1 The included processes and elements in view of nutrient availability and pH

Basically both modelling systems include most of the relevant processes. The main lacking processes or elements are:

- P – only partly included both models
- Cation exchange – only fully included in SUMO-VSD$^+$

**The role of phosphorus in nutrient availability:** To include chemical aspects of P is not a complicated task for oxic (dry) systems. Descriptions, and the corresponding data, to do this are available for agricultural systems (see e.g. Van der Salm *et al.*, 2016), while limited data are also available for natural systems (De Vries & Leeters, 2001). However, this is only valid for oxic (dry) systems. Furthermore, the model validation presented in Van der Salm *et al.* (2016) has been limited to agricultural systems and it appeared that the included models did perform well under P excess, but not under P limited circumstances. For anoxic (wet) systems it is necessary to include reductions processes, which makes it more complicated The main challenge will be how to include the P availability. If we use mineralisation plus deposition as an indicator, than the inclusions of the soil chemical processes is of minor importance. Most of the P will be turned over though mineralisation. On the other hand, the adsorbed P might be a limiting factor for species diversity; see e.g. Sival and Chardon (2002), who showed that there is a relation between Pw and P-Al and biomass production and the N:P ratio in the vegetation.

**The role of cation exchange:** For the regulation of the pH, especially within the pH range 4.5-6.5, cation exchange is the most prominent process. So, it is obvious that there is a clear need to include cation exchange. Inclusion of cation exchange by using ORCHESTRA is, however, cumbersome (huge computational load limits the applicability). Beyond the relevance of inclusion as such, also how cation exchange is modelled is relevant. E.g. using either Kerr, Gapon or Gaines Thomas relationships. Validation on empirical pH-Base saturation relationships can help to identify the most suitable relationship.

## 4.2 The role of the calculation order of the modelled processes

The most notable difference is that PROBE calculates nitrification and denitrification before uptake, whereas VSD calculates uptake first. This means that PROBE treats uptake as a slower, less efficient, process than nitrification and denitrification, while VSD+ assumes that uptake takes place first. The consequence of this choice on N availability and related cation availability and pH, depends on the used calculation time-step. At a larger time-step (VSD+), the process-order has a larger impact than at a smaller time-stem (PROBE).

## 4.3 The used spatial and temporal scale

Effect of spatial resolution can be distinguished in resolution in the vertical direction and the horizontal direction. Regarding the vertical resolution the VSD assumes one soil homogeneous compartment for the root zone as a whole, rather than the top soil where most of the fine roots occur. This assumption implies that the calculated concentrations refer to the bottom of the root zone. Generally, there is a strong gradient in soil solution chemistry and fine root distribution with depth. pH and Al concentrations generally decrease with depth, as most of the fine roots occur in the top soil. The PROBE model, however, does include multiple layers and is capable to simulate gradients with depth. However, the regional applicability (the horizontal direction) of this model is low due to limited availability of regional process parameters.

The two models also differ in temporal scale yearly (VSD+) versus daily (PROBE). The influence of the chosen temporal scale, daily versus yearly mean, can particularly strong for the $NO_3$, $NH_4$ and base cations concentrations, which are strongly influenced by seasonal processes as nutrient uptake and mineralisation, which is especially the case in the upper 30 cm.

Both a high spatial and temporal resolution are especially needed in nature areas with small rain water lenses floating upon upwelling alkaline groundwater. Such nature reserves exhibit strong vertical and horizontal gradients in groundwater chemistry, which is one of the explanations for their high species richness (Cirkel *et al.*, 2014a; Cirkel *et al.*, 2014b). These areas often harbour habitat types and plant species that are highly protected by both national and international legislations. To account for the dynamics of the rainwater lenses in such areas, and for the sensitivity of the vegetation to subtle changes in weather conditions and water management, modelling with fine spatial and temporal resolutions is a prerequisite. This of course requires huge computation times. To avoid such a time consuming effort, process models can be used to generate easy-to-use repro-functions (Bartholomeus & Witte, 2013; Cirkel *et al.*, 2016b). Another option might be to drastically schematize and simplify processes (De Haan *et al.*, 2010; Stofberg *et al.*, 2017).

## 4.4 Challenges in definition of nutrient availability

One of the biggest challenges in making a robust prediction of vegetation response is to improve the poor relationship between the indicator value for nutrient availability, Nm, and the actual nutrient availability in soil, and the mismatch between these two definitions. Unlike soil moisture and soil acidity, nutrient availability cannot be easily judged in the field and therefore the above-ground productivity of the vegetation is used as the visible proxy of Nm. However, the productivity of vegetation is not only influenced by nutrient availability but also by soil moisture and acidity. On top of that, biological factors also influence productivity: plants may produce root exudates to change pH around the roots or produce oxygen to change redox status, so that nutrients become more available for plants on that micro scale. Runhaar tackled this issue by defining Nm as ‘potential plant productivity based on nutrient availability’. In this way, the effects of other abiotic factors (e.g. moisture and acidity) are in principle eliminated from the expert judgement of Nm. Still, the fact that Nm was more strongly related to above-ground biomass production than to any measures of nutrient availability (Fujita, unpublished) indicates that the bias in expert judgement hampers the clear relationship between Nm and soil nutrient availability.

At this moment we do not have a better alternative to replace Nm; quantitative species traits, such as leaf nutrient concentrations and SLA, failed to exhibit a better correlation with soil nutrient measures. Therefore, in the context of WWN, we strive to find the best measure of nutrient availability in soil which matches what Nm represents.

In that regard, making a clear definition of nutrient availability in soil is another challenge. In this report, we came up with a theoretically plausible measure of nutrient availability for plants, i.e. sum of net N mineralization, N deposition, asymbiotic N fixation, minus denitrification. However, there are still rooms to improve the definition and interpretation. For example, which time scale should we use? We choose the time scale of one year because the study of Fujita et al (2013) indicated that time scale had only minor influence on the relationships between Nm and nutrient availability. However, these relationships were obtained in (near-) equilibrium ecosystems, whereas under climate change scenarios inter-annual relationships may have much stronger influence on the relationships. In addition, one will expect a time-lag in plant response under changing climate, because vegetation types do not instantaneously respond to the changes in nutrient availability in soil. Should we then use moving average of nutrient availability to have a better relationship between Nm and nutrient availability? If so, which time span should we take into account? In phase 2, we need to keep exploring the best definition of nutrient availability by means of comparing the model output with field observation from the available dataset.

### 4.5 Model initialization

The two models reviewed in this study use different initialization scheme for obtaining initial sets of state variables. Especially when the goal of modelling exercise is to predict (regional) spatial distribution of vegetation types In an equilibrium state, proper initialization of the model state variables (among others, C pool, N pool) is the key for successful prediction. The initialization schema is disconnected from the dynamic modelling processes. Based on the overview given in Section 2.2 and Section 2.3, we should combine our best knowledge and data to improve the initialization scheme to provide the proper ‘starting points’ to the model, irrespective of which model framework is chosen.

When the goal of modelling exercise is to predict dynamic changes of nutrient availability or soil acidity under changing environment, then the model initialization of state variables becomes of relatively less importance. Instead, proper inclusion of feedback effects between soil, water, and plants plays much more importance. Especially for predicting nutrient availability, the balance between the effects of abiotic factors (e.g. temperature, soil moisture) on plant growth, plant death, and on soil organic matter decomposition determine how much nutrients accumulate in soil. These effects are often counteracting: for example, high temperature and high moisture speeds up soil decomposition (i.e. less accumulation) and they stimulate plant uptake (i.e. less accumulation) whereas they also increase litter input to soil (i.e. more accumulation). This means that subtle errors in parametrization for these processes can mislead the overall effects of climate change on nutrient availability. PROBE model is equipped to simulate these chains of feedback effects under changing environment, while VSD+ is not. If VSD+ is coupled with SUMO, then they are also able to handle the feedbacks. However, for both PROBE and VSD+ coupled with SUMO, it is a big challenge to properly parametrize all the equations which influence the feedback chains. In phase 2, efforts are needed to examine the uncertainties around the parametrization and to quantify how the error propagates in the course of model simulation period. Further, to evaluate plausibility of the model to simulate dynamic changes in nutrient availability, model validation should be conducted using time-series data under experimentally manipulated abiotic conditions, such as those of lysimeter study in Hoge Veluwe.

## 4.6 The availability of data

One of the aims of the next phase will be the development of a nationwide applicable and flexible model to model the pH and nutrient availability adequately. Therefore are several datasets were inventoried for either parametrization or validation. A total number of nine data sets were inventoried to be used for parametrization. For the validation ten time series were inventoried. However, not all of these dataset are suitable for model validation, e.g. due to incompleteness or a too short monitoring period. About four time series seems of appropriate completeness enough to be suitable to be used for model comparison and validation. Another shortcoming is that the majority of this dataset is focused on the drier terrestrial ecosystems, so the wetter systems cannot be adequately addressed.

The most promising datasets seems to be:

- For grassland: Veenkampen (long-term monitoring site including interaction with groundwater)
- For forest: Speuld (This is one of the very view sites in the Netherland with a long-term monitoring record. Furthermore, various model applications has been performed for this site, e.g. SMART2)
- Lysimeter site Hoge Veluwe (relevant in view of the BTO-project)
- Solling (A long-term monitoring record for a Spruce forest in Germany. For this site the VSD+ model has already been applied)

# 5 Conclusions and recommendations

## 5.1 Conclusions

- Main similarities are:
    - Overall the same process are included in both models.
    - In general the used reduction function for environmental factors in both models are quite comparable. Differences exist for the effect of soil and litter quality and the effects of soil available N.

- Main differences are:
    - Scale, both temporal (daily versus yearly) and spatial (plot versus regional; one-layer versus multi-layer). Where PROBE is operating at a daily time scale for multi-layer soil profiles and VSD+ at a yearly time scale and at a regional spatial scale.
    - The principal difference between the two model chains is the level of detail used in the soil chemistry and soil hydrology part. Where PROBE is much more detailed in view of soil chemistry and soil hydrology.
    - Effects of nutrient limitation and C:N:P stoichiometry on plant growth and decomposition are only explicitly included in PROBE.
    - PROBE is rather complex with many input (parameter) values and requires a high computational load whereas the opposite is true for VSD+.

- Consequences of differences:
    - Some of the effects of environmental factors are not included in a model but in the other (e.g. temperature effect on plant death, pH effect on denitrification) or modelled differently. However, these reduction equations can be easily added or replaced without changing model structure.
    - PROBE takes more process-based approach to reflect the effects of environmental factors. These (temporal) effects are not easily replaced since it requires changes in model structure (i.e. increases in state variables) or requires different time scale.
    - A small time step, enable to include temporal aspects, such as seasonality, effect of short weather events, inter-annual management options and a feedback between plant, soil, and hydrology.
    - The pH module PROBE is not robust for all combinations of input value
    - VSD+ does not include redox-processes.
    - The applicability is rather demanding for PROBE, whereas VSD+ is rather easy to apply.

## 5.2 Recommendations

Based on the performed analyses and comparisons we come to the following recommendations in order to derive a robust and adequate pH and nutrient availability module for the WWN:

- pH: improve the relationship between pH and base saturation, which is crucial for the pH prediction between 4.5 and 6.5, which is a common pH for groundwater influenced ecosystems. Furthermore, include the role of upward seepage, both in view of quantity and quality.

- N availability: N transformations such as mineralisation, nitrification and denitrification are strongly influenced by soil moisture and pH. These relationships are crucial for an adequate prediction of the N leaching and N availability. Since the relationships currently are not always scientifically sound, it is recommended to improve these relationships.
- P availability: since P availability is also relevant in view of plant species diversity it is recommended to include P availability in the WWN. However, it is too complicated and not realistic to include a process based P availability module. Therefore, we recommend to derived relationships between solid phase or adsorbed P (such as Pox, Pw) and biomass production.

# 6 Literature

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# Appendix I Comparison of model input data

Input values for soil module and pH module of VSD+ are separately shown for the sake of comparison with CENTURY-SWAP-ORCHESTRA, although these two modules are integrated in VSD+. The descriptions of PROBE model are of PROBE-2.2 (for pH) and PROBE-3 (for the rest). Input values are divided into: initial values of state variables, site-specific input values, vegetation-specific parameters (for which different default values are set for each vegetation type or species), fixed parameters (i.e. those which do not vary between sites nor vegetation types), and input values which are computed in other model modules.

| | **PROBE (CENTURY-SWAP-ORCHESTRA)** | **VSD+** |
|---|---|---|
| General | · Calculation period (begin and end date)<br>· Thickness of each soil layer (cm) | · Site information, title above the produces chart;<br>· Calculation period (begin and end year);<br>· Thickness of soil compartment (m); |
| Model options | · Growth option for plant module: Trees, grasses, or trees + grasses | · Cation exchange model option (Gaines-Thomas model (1) or Gapon model (2)<br>· Organic acid dissociation model option; Oliver model (0), mono-protic organic acid (1) or none (-1);<br>· Parameters for organic acid dissociation model; |
| Input (soil module) | 'CENTURY' (SOM module)<br>[Initial values of state variables]<br>· Initial C content in top soil (gC/m2)<br>· Initial N content in top soil (gN/m2)<br>· Initial concentrations of NO3 and NH4 in top soil layer (gN/m2)<br>· Initial concentrations of total mineral N (NO3+NH4) in the second and third soil layer (gN/m2)<br>· Initial C content in plant litter (gC/m2)<br>· Initial content of dead wood biomass (for forest only) | 'VSD+'<br>[Initial values of state variables]<br>· Initial amount of C in top layer (g/m2);<br>· Initial C:N ratio in topsoil (g/g);<br>· Initial concentration of NO3- and NH4+ (eq/m2) |

|  |  |  |
|---|---|---|
|  | [Site-specific input values]<br>· Atmospheric N deposition (wet + dry) (gN/m2/yr)<br>· Non-symbiotic biological N fixation (gN/m2/yr)<br>· Volumetric water content at saturation ($\theta_{sat}$), field capacity ($\theta_{fc}$), and wilting point ($\theta_{wilt}$)<br>· Soil clay, silt, and sand content (fraction)<br>· Lignin content in shoots and roots (fraction) (This can also be approximated based on average annual precipitation (mm/year))<br>· Relative root density in each soil layer (fraction between 0 and 1) | [Site-specific input values]<br>· Deposition of $NO_x$ and $NH_3$ (eq/m2/yr);<br>· Nitrogen fixation (eq/m2/yr)<br>· Volumetric water content at saturation ($\theta_{sat}$), field capacity ($\theta_{fc}$), wilting point ($\theta_{wilt}$), and at a pressure of -1 bar ($\theta_{P=-1 bar}$)<br>· Clay content of the soil (%);<br>· Quality index of litterfall (-) for the RothC model<br>· Yearly air temperature (˚C). Based on either daily, weekly or monthly data a yearly a reduction fraction is derived for each year. |

| | | |
|---|---|---|
| | [Fixed parameters]<br>· Maximum decomposition rate for each SOM pool (day-1) ('dec1' – 'dec5'; and for forests, 'decw1', 'decw2', 'decw3' additionally)<br>· Coefficient values for reduction function of soil temperature on decomposition rate ('teff(1..4)')<br>· Coefficient values for reduction function of moisture on decomposition rate<br>· Coefficient values for reduction function of texture on decomposition rate ('peftxa', 'peftxb')<br>· Coefficient values for reduction function of lignin on decomposition rate ('pligst(1..2)')<br>· Coefficient values for reduction function of texture on microbial yield efficiency | [Fixed parameters]<br>· Maximum decomposition rate of each C pool (yr-1) ($k_{DPM,ref}$, $k_{RPM,ref}$, $k_{BIO,ref}$, $k_{HUM,ref}$);<br>· Coefficient values for reduction function of moisture on mineralisation rates<br>· Coefficient values for reduction function of temperature on mineralisation rates<br>· Coefficient values to function of clay on fraction of decomposed C converted to CO2 |
| | · Maximum nitrification rate (day-1)<br>· Coefficient values for reduction function of soil pH on nitrification rate<br>· Coefficient values for reduction function of soil temperature on nitrification rate<br>· Coefficient values for reduction function of soil moisture on nitrification rate<br>· Coefficient values for function of labile C on denitrification rate<br>· Coefficient values for function of nitrate on denitrification rate<br>· Coefficient values for reduction function of soil moisture on denitrification rate | · Nitrification rate at reference temperature of 10° (yr-1);<br>· Coefficient values for reduction factor of moisture and temperature on nitrification rates<br>· Denitrification rate at reference temperature of 10° (yr-1);<br>· Coefficient values of reduction factor of moisture and temperature on denitrification rates; |
| | · Minimum and maximum C:N ratios of surface microbe, active, slow, and passive pools ('pcemic(1..2,1)' , 'varat1' – 'varat3')<br>· C:N ratio of structural pools ('rcestr(1)')<br>· Coefficient values to determine the effect of soil texture on flow rates of active pool into slow and passive pools ('ps1s3(1..2)')<br>· Coefficient values to determine the effect of lignin on flow rates from surface structural pool into surface microbe and slow pools ('spl(2)')<br>· Coefficient values to determine the effect of lignin on flow rates from belowground structural pool into active and slow pools<br>· Coefficient values for function of lignin and nitrogen content on division of plant residues into metabolic and structural pools<br>· Initial division of C into different soil pools (fractions). This is related to initialization of C pools. | · C:N ratios of three C pools (BIO, RPM, and IOM)<br>· Fraction of decomposed C that is transferred to the BIO pool ($fr_{BIO}$) |

| | | |
|---|---|---|
| | [Input from other model module]<br>· Daily water flow between layers (cm/d)<br>· Daily soil volumetric water content (cm3/cm3)<br>· Daily soil temperature (˚C)<br>· Daily plant demand of N for potential production (gN/m2/d)<br>· Daily plant residue input (for each plant component) in terms of C and N (gC/m2/d or gN/m2/d)<br>(· Soil pH) | [Input from other model module]<br>· Percolation (i.e. the water that is leaving the soil compartment) (m/yr);<br>· Volumetric water content (m3/m3). Based on either daily, weekly or monthly data a yearly a reduction fraction is derived for each year.<br>· Total plant uptake of N (eq/m2/yr);<br>· Litter fall C and N (g/m2/yr);<br>· Soil pH |
| Input (pH module) | 'ORCHESTRA'<br>[Initial values of state variables]<br>· initial concentrations of 'master' species of cations and anions (H+, Cl-, HCO3-, NO3-, SO42-, PO43-, Ca2+, Mg2+, Na+, K+, Mn2+, NH4+,CO2[g], in mol/L) (speciation according to ORCHESTRA database Minteqv4) | 'VSD+'<br>[Initial values of state variables]<br>· Fraction (0-1) of Ca in the parent material of a calcareous soil;<br>· Initial base saturation (fraction 0-1) or separately initial saturation of Ca, Mg and K;<br>· Initial concentration of cations and anions, i.e. H+, SO42-, NO3-, Cl-, HCO3-, Org-, Ca2+, MG2+, K+, Na+, Al3+, NH4+ (eq/m2) |
| | [Site-specific input values]<br>· Chemical composition of groundwater (pH, Cl-, HCO3-, NO3-, SO42-, PO43-, Ca2+, Mg2+, Na+, K+, Mn2+, NH4+,CO2[g], in mol/L)<br>· Chemical composition of rainwater (pH, Cl-, HCO3-, NO3-, SO42-, PO43-, Ca2+, Mg2+, Na+, K+, Mn2+, NH4+,CO2[g], in mol/L)<br>· Soil substrate density (g/cm3) for each soil layer<br>· Porosity (cm3/cm3) for each soil layer<br>· Clay (kg/kg) for each soil layer<br>· Soil organic matter (kg/kg) for each soil layer<br>· Total calcium content of the soil (mol/kg) (inc. adsorbed/calcite/pore water Ca)<br>· Iron (hydro)oxide + aluminium oxide (kg/kg) for each soil layer<br>· Gibbsite Al(OH)3 (kg/kg) for each soil layer<br>· Calcite CaCO3 (kg/kg) for each soil layer<br>· CEC for each soil layer (approximated from clay, SOM, pH) | [Site-specific input values]<br>· Deposition of SO2, Ca, Mg, K, Na and Cl (eq/m2/yr);<br>· Uptake efficiency of available N (fraction between 0-1), i.e. is the fraction of the N deposition that is<br>available for uptake.;<br>· Weathering rates for Ca, Mg, K and Na (eq/m3/yr);<br>· Concentration of organic acids (m*DOC) (mol/m3); either a constant value or a time series with yearly values.<br>· Bulk density (g/$cm^3$)<br>· Average potential cation exchange capacity (CEC) of the soil (meq/kg);<br>· log10 of selectivity constant for Al-BC exchange;<br>· log10 of selectivity constant for H-BC exchange;<br>· log10 of Al equilibrium constant ((mol/l)1-expAl); |

| | | |
|---|---|---|
| | [Fixed parameters]<br>· Maximum weathering rate of silicates (molc/m2/s/cm)<br>· Coefficient values for function of pH on weathering rate of silicates<br>· Coefficient values to determine root respiration as a function of transpiration | [Fixed parameters]<br>· CO2 pressure in the soil solution (given as a multiple of pCO2(atm) in air);<br>· Exponent in [Al] = KAlox*[H]expAl (>0); default is 3 (gibbsite equilibrium); |
| | [Input from other model module]<br>· Daily soil volumetric water content (cm3/cm3) and water flow between layers (cm/d)<br>· Daily soil temperature (˚C) | [Input from other model module]<br>· Percolation (i.e. the water that is leaving the soil compartment) (m/yr);<br>· Volumetric water content (m3/m3);<br>· Concentration of NO3- and NH4+ (eq/m2)<br>· Net plant uptake Ca, Mg and K (eq/m2/yr); |
| Input (plant module) | 'CENTURY' (plant module)<br>[Initial values of state variables]<br>· Initial above-ground plant biomass (g/m2)(for grassland)<br>· Initial biomass of 5 plant components: leaves, fine roots, fine branches, large woods, and coarse roots (for forest) | 'Growup'<br>[Initial values of state variables]<br>· The initial distribution of the stem volumes of the various tree species (for uneven aged forests only) |
| | [Site-specific input values]<br>· Mowing rate (fraction between 0-1) (for grassland only) | [Site-specific input values]<br>· Year of planting (even aged forests only),<br>· Fraction of biomass that is removed by thinning (%), and the year in which the action take place, and which residues are left at the plot<br>· Year of clear cut, and which residues are left at the plot. |

| | | |
|---|---|---|
| | [Vegetation-specific parameters: Forests]<br>(Default values are set for each forest type, but can be modified by the user)(Items with * are also common for the grassland version) | [Vegetation-specific parameters]<br>(Default values are set for each tree species, but can be modified by the user) |
| | · Maximum gross forest production rate (g biomass/m2/day) ('prdx(2)')<br>· maximum net production of trees (g C/m2/day) ('prdx(3)')<br>· *Coefficient values for reduction function of soil temperature on plant growth ('ppdf(1..4)') | · Forest growth rate for different age classs (m3/ha/y) (for even aged forests)<br>· Maximum tree growth rate (m3/ha/y) (for uneven aged forests)<br>· Coefficient value to determine effect of competition on growth rate (for uneven aged forests) |
| | · Coefficient to determine LAI effects on tree production ('laitop')<br>· C allocation fraction of new production to different forest compartments, for juvenile forest and for mature forest ('fcfrac(1..5,1)', 'fcfrac(1..5,2)') | · Biomass expansion factors (BEFs) for each tree compartment and for each age class. (Default values are set for different regions ) |
| | · Month-specific death rate of leaves (fraction /day) ('leafdr(1..12)')<br>· Death rate for each forest components except for leaf (fraction/day)('wooddr(2..5)') | · Turnover rates of each tree compartments (yr-1) |
| | · *Fall rate of standing dead (fraction /day) ('fallrt') | · Carbon content in biomass (%)<br>· Wood density (g/cm3) |
| | · Maximum and minimum C:N ratio of each tree compartment ('cerfor(1,1..5,1)', ('cerfor(2,1..5,1)' ) | · Nutrient (Ca, Mg, K) contents of each tree compartments (%).<br>· Maximum and minimum N content in leaves (%)<br>· Coefficient to determine the effect of N deposition on N content in leaves |
| | · *Maximum level of N fixed per C fixed (gN/gC) ('snfxmx')<br>· *Proportion of plant species associated with symbiotic N fixers (fraction in 0-1)<br>· Coefficients to approximate LAI from large wood ('maxlai', 'klai')<br>· Coefficient controls the ratio of sapwood to total stem wood ('spak')<br>· Lignin fraction for each forest component (fraction)('wdlig(1..5)') | |

| | | |
|---|---|---|
| | [Vegetation-specific parameters: Grasslands]<br>(Default values are set, but can be modified by the user)<br>· Maximum growth rate (gC/m2/day) ('prdx(1)')<br>· *Coefficient values for reduction function of soil temperature on plant growth (‘ppdf(1..4)’)<br>· The amount of the shading materials (gC/m2) with which production is reduced to half maximum (‘biok5’)<br>· Coefficient values to determine lignin content as a function of annual rainfall (‘fligni’)<br>· Maximum shoot and root death rate (fraction/day) (‘fdeth(1)’, ‘rdr’)<br>· Shoot death rate of the senescence month (fraction) ) (‘fdeth(2)’)<br>· Extra death rate of shoot due to shading (fraction /day) ) (‘fdeth(3)’)<br>· Threshold value of plant biomass above which shading effect on shoot death is induced (g/m2) (‘fdeth(4)’)<br>· *Fall rate of standing dead (fraction /day) (‘fallrt’)<br>· *Maximum level of N fixed per C fixed (gN/gC) (‘snfxmx’)<br>· *Proportion of plant species associated with symbiotic N fixers (fraction in 0-1)<br>· Maximum and minimum C:N ratio of root (ratio) (‘prbmn’, ‘prbmx’)<br>· Maximum and minimum C:N ratio of shoot when biomass is nearly zero (ratio) (‘pramn(1..3,1)’, ‘pramx(1..3,1)’)<br>· Maximum and minimum C:N ratio of shoot when biomass reaches threshold (ratio) (‘pramn(1..3,2)’, ‘pramx(1..3,2)’)<br>· Threshold value of shoot biomass when C:N ratio reaches the maximum (g biomass/m2) (‘biomax’) | |

| | | |
|---|---|---|
| | [Fixed parameters]<br>· Coefficient values for reduction function of soil moisture on plant growth<br>· Coefficient values for function of soil moisture on plant death<br>· Coefficient values to determine the effect of root biomass on the fraction of soil mineral N available for plants ('rictrl', 'riint')<br>· Coefficient values to determine shoot:root ratio of newly-produced biomass based on annual precipitation ('agppa', 'agppb', 'bgppa', 'bgppb') | |
| | [Input from other model module]<br>· Daily soil mineral N availability in top soil (gN/m2)<br>· Daily soil volumetric water content (cm3/cm3) [when coupled with hydrological module of CENTURY]<br>· Potential and actual transpiration (cm/d) [when coupled with SWAP]<br>· Daily soil temperature (°C) | [Input from other model module]<br>none |
| | | 'SUMO'<br>[Initial values of state variables]<br>· Initial biomass per organ and per vegetation structure type. For the standard regional version the initial values per vegetation structure type and age class are provide by the model. For standalone application (e.g. in combination with VSD+) these values must be provide by the user.<br>· Initial N content per organ and per vegetation structure type<br>· Vegetation structure type (one of 23 types)<br>· Age of the vegetation (yr) |

| | | |
|---|---|---|
| | | [Site-specific input values]<br>· Fertilisation (ton N · ha-1 · yr-1)<br>· Management (no management or one of 10 options)<br>· Frequency of management (yr) (management options occurring once in a period of serval years)<br>· Frequency of mowing (times · yr-1) (management options occurring more than once per years)<br>· Cutting cycle period and the percentage of thinning per thinning cycle For the regional version predefined values are include in the model. For standalone application (e.g. in combination with VSD+) these values must be provide by the user.<br>· Pioneer tree species (none, or one of 23 tree species)<br>· Climax tree species (none, or one of 23 tree species) |
| | | [Vegetation-specific parameters]<br>(these values are different per tree species for forests, or per vegetation type for the functional types grasses and herbs, dwarf shrubs and shrubs)<br>· Division of new biomass and nitrogen over the organs (fraction)<br>· Added amount of seed biomass in the system<br>· Fraction of dead biomass per organ<br>· Light extinction factor, i.e. the fraction of light remaining after interception in the canopy.<br>· Minimum and maximum N content (%), i.e. the boundaries between the actual N content may vary.<br>· Minimum and maximum P content (%), i.e. the boundaries between the actual P content may vary.<br>- Coefficient values to determine the effect of N deposition on N content in leaves<br>· Maximum growth rate (ton/ha/yr)<br>· Coefficients for the effect of biomass increment on tree growth (m/yr)<br>· Potential transpiration per vegetation type (mm/yr) |

| | | |
|---|---|---|
| | | [Fixed parameters]<br>· Minimum of biomass that is required per organ before grazers can eat from the biomass (ton/ha)<br>· The amount of biomass eaten by each grazer, the fraction that become excreted, and the N and P contents of the faeces and urea<br>· Fraction of N that is reallocated depending on the N content of the organ per organ |
| | | [Input from other model module]<br>· N availability in soil (an extended version also uses P, Ca, Mg and K availability)<br>. Mean spring water level in cm below surface<br>· Temperature<br>· $CO_2$ |

# Appendix II Available dataset for parameterization

TABLE 7 DESCRIPTION OF DATASET WITH FOREST STANDS SAMPLED IN 1990

| **Monitoring Characteristics** | **Type of measurement** | **Elements included** |
|---|---|---|
| Reference | De Vries and Leeters (2001) | |
| Country | Netherlands | |
| Ecosystem/vegetation | Forest | |
| Period | 1990 | |
| Soil type | Non-calcareous sand | |
| Amount of locations | 150 | Non-calcareous sand |
| Sample depth | Litter | |
| | 0-30 cm | |
| | 30-60 cm | |
| | 60-100 cm | |
| Duplicates | 20 subsamples mixed to one | |
| Soil Parameters | Soil contents (solid phase) | C, N, P, K, Ca, Mg, S (litter) |
| | | C, N, P (mineral) |
| | Soil solution concentrations | pH, Al, Fe ,K, Ca, Mg, K, Na, |
| | | $NH_4$, $NO_3$, $SO_4$, Cl, $RCOO_-$ |
| | CEC | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$ |
| | Oxalate extractable | Al, Fe, P |
| Carbon and Nutrient pools | | C, N, P |
| Vegetation parameters | Nutrient contents in foliage | |
| Species composition | No | |

TABLE 8 DESCRIPTION OF DATASET WITH FOREST STANDS TO DEFINE THE STARTING POINT FOR ACIDIFICATION RESEARCH

| **Monitoring Characteristics** | **Type of measurement** | **Elements included** |
|---|---|---|
| Reference | De Vries *et al.* (1995) | |
| Country | Netherlands | |
| Ecosystem/vegetation | Forest | |
| Period | 1992 | |
| Soil type | Non-calcareous sand | |
| Amount of locations | 12 | |
| Sample depth | Litter | |
| | 0-10 cm | |
| | 10-30 cm | |
| | 30-60 cm | |
| | 60-100 cm | |
| Duplicates | 20 subsamples mixed to one | |
| Soil Parameters | Texture | |
| | Soil contents (solid phase) | C, N, P, K, Ca, Mg, Na, S |
| | Soil solution concentrations | pH, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$, $NO_3$, $SO_4$, Cl, $H_2PO_4$, $RCOO_-$ |
| | CEC | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$ |
| | Oxalate extractable | Al, Fe, P |
| Carbon and Nutrient pools | | C, N, P |
| Vegetation parameters | Nutrient contents in foliage | |
| Species composition | | |

TABLE 9 DESCRIPTION OF DATASET WITH DUNE LOCATIONS, SAMPLED IN 1992

| **Monitoring Characteristics** | **Type of measurement** | **Elements included** |
|---|---|---|
| Reference | (De Vries, 1993) | |
| Country | Netherlands | |
| Ecosystem/vegetation | Dunes, grassland and deciduous forest | |
| Period | 1992 | |
| Soil type | Calcareous and non-calcareous sand | |
| Amount of locations | 48 | |
| Sample depth | Litter | |
| | 0-10 cm | |
| | 10-30 cm | |
| | 30-60 cm | |
| Duplicates | 20 subsamples mixed to one | |
| Soil Parameters | Soil contents (solid phase) | C, N, P, K, Ca, Mg, S (litter)<br>C, N, P (mineral) |
| | Soil solution concentrations | pH, Al, Fe , Mn, K, Ca, Mg, Na, $NH_4$, $NO_3$, $SO_4$, Cl |
| | CEC | H, Al, Fe ,Mn, K, Ca, Mg, K, Na |
| | Oxalate extractable | Al, Fe, P |
| Carbon and Nutrient pools | | C, N, P |
| Vegetation parameters | Nutrient contents in foliage | |
| Species composition | | |

TABLE 10 DESCRIPTION OF DATASET WITH FOREST STANDS ON LÖSS SOILS, SAMPLED IN 1992

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Klap *et al.* (1999b) | |
| Country | Netherlands | |
| Ecosystem/vegetation | Forest | |
| Period | 1992 | |
| Soil type | Löss | |
| Amount of locations | 40 | |
| Sample depth | Litter | |
| | 0-10 cm | |
| | 10-30 cm | |
| | 30-60 cm | |
| | 60-100 cm | |
| Duplicates | | |
| Soil Parameters | Soil contents (solid phase) | C, N, P, K, Ca, Mg, S (litter)<br>C, N, P (mineral) |
| | Soil solution concentrations | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$, $NO_3$, $SO_4$, Cl, $RCOO_-$ |
| | CEC | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$ |
| | Oxalate extractable | Al, Fe, P |
| Carbon and Nutrient pools | | C, N, P (all) Ca, Mg, K, Fe, Mn (subset of 10) |
| Vegetation parameters | Nutrient contents in foliage | |
| Species composition | | |

TABLE 11 DESCRIPTION OF DATASET WITH FOREST STANDS ON CLAY SOILS

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Klap *et al.* (1999b) | |
| Country | Netherlands | |
| Ecosystem/vegetation | Forest | |
| Period | 1993 | |
| Soil type | Clay | |
| Amount of locations | 30 | |
| Sample depth | Litter | |
| | 0-10 cm | |
| | 10-30 cm | |
| | 30-60 cm | |
| | 60-100 cm | |
| Duplicates | | |
| Soil Parameters | Soil contents (solid phase) | C, N, P, K, Ca, Mg, S (litter)<br>C, N, P (mineral) |
| | Soil solution concentrations | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$, $NO_3$, $SO_4$, Cl, $RCOO_-$ |
| | CEC | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$ |
| | Oxalate extractable | Al, Fe, P |
| Carbon and Nutrient pools | | C, N, P (all) Ca, Mg, K, Fe, Mn (subset of 10) |
| Vegetation parameters | Nutrient contents in foliage | |
| Species composition | | |

TABLE 12 DESCRIPTION OF DATASET WITH FOREST STANDS ON PEAT SOILS

| **Monitoring Characteristics** | **Type of measurement** | **Elements included** |
|---|---|---|
| Reference | Klap *et al.* (1999b) | |
| Country | Netherlands | |
| Ecosystem/vegetation | Forest | |
| Period | 1993 | |
| Soil type | Peat | |
| Amount of locations | 30 | |
| Sample depth | Litter | |
| | 0-10 cm | |
| | 10-30 cm | |
| | 30-60 cm | |
| | 60-100 cm | |
| Duplicates | | |
| Soil Parameters | Soil contents (solid phase) | C, N, P, K, Ca, Mg, S (litter) |
| | | C, N, P (mineral) |
| | Soil solution concentrations | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$, $NO_3$, $SO_4$, Cl, $RCOO_-$ |
| | CEC | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$ |
| | Oxalate extractable | Al, Fe, P |
| Carbon and Nutrient pools | | C, N, P, Ca, Mg, K, Fe, Mn |
| Vegetation parameters | Nutrient contents in foliage | |
| Species composition | | |

TABLE 13 DESCRIPTION OF DATASET WITH MEASUREMENTS IN DRENTSE AA AREA

| **Monitoring Characteristics** | **Type of measurement** | **Elements included** |
|---|---|---|
| Reference | Klap *et al.* (1999a) | |
| Country | Netherlands, Drentse AA | |
| Ecosystem/vegetation | Different | |
| Period | 1994 | |
| Soil type | Sand (41), Peat (15) and clay (4), arable (3) | |
| Amount of locations | 63 (50 sampled, 13 in other sets) | |
| Sample depth | Litter (only forest and heath where available) | |
| | 0-10 cm | |
| | 10-30 cm | |
| | 30-60 cm | |
| | 60-100 cm | |
| Duplicates | 20 subsamples mixed to one | |
| Soil Parameters | Soil moisture content | |
| | Bulk density | |
| | Soil contents (solid phase) | C, N, P, pH ($H_2O$ and KCl) |
| | Soil solution concentrations | pH, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$, $NO_3$, $SO_4$, Cl, $RCOO_-$ EGV |
| | CEC | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$ |
| | Oxalate extractable | Al, Fe, P (not in litter) |
| Carbon and Nutrient pools | | C, N, P |
| Vegetation parameters | Nutrient contents in foliage | |
| Species composition | | |

TABLE 14 DESCRIPTION OF DATASET WITH RESAMPLING OF FOREST STANDS ON SANDY SOILS

| **Monitoring Characteristics** | **Type of measurement** | **Elements included** |
|---|---|---|
| Reference | Leeters and de Vries (2001) | |
| Country | Netherlands | |
| Ecosystem/vegetation | Forest | |
| Period | 1995 | |
| Soil type | Non-calcareous sand | |
| Amount of locations | 200 | |
| Sample depth | Litter | |
| | 0-10 cm | |
| | 10-30 cm | |
| Duplicates | 10 (litter) or 25 (mineral) subsamples mixed to one | |
| Soil Parameters | Soil contents (solid phase) | C, N, P, K, Ca, Mg, S (litter) |
| | | C, N, P (mineral) |
| | Soil solution concentrations | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$, $NO_3$, $SO_4$, Cl, $RCOO_-$ |
| | CEC | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$ (only 0-10 cm), 0-30: acidity |
| | Oxalate extractable | Al, Fe, P |
| Carbon and Nutrient pools | | C, N, P |
| MSW | Nutrient contents in foliage | |
| Vegetation parameters | | |
| Species composition | | |

TABLE 15 DESCRIPTION OF DATASET HUMBASE (BETWEEN BRACKETS THE NUMBER OF SAMPLES)

| **Monitoring Characteristics** | **Type of measurement** | **Elements included** |
|---|---|---|
| Reference | Van Delft (2001); (Van Delft, 2013) | |
| Country | Netherlands | |
| Ecosystem/vegetation | Grassland, heath and forest | |
| Period | 1990 – 2013 | |
| Soil type | Different soil types | |
| Amount of locations | 296 | |
| Sample depth | 0-10 (67) | |
| | 0-15 (14) | |
| | 0-20 (40) | |
| | 0-25 (83) | |
| | 0-30 (15) | |
| | Other depths (78) | |
| Duplicates | No | |
| Soil Parameters | Soil contents (solid phase) | C, N, P (mineral) |
| | | pH-$H_2O$ (146) pH-KCl (596) |
| | CEC (474) | H, Al, Fe ,K, Ca, Mg, K, Na, $NH_4$ (only 0-10 cm), 0-30: acidity |
| | Oxalate extractable | Al (240), Fe (218), P (235) |
| Carbon and Nutrient pools | | C (41), humus (666), N (540), P (475) |
| Vegetation parameters | | |
| Species composition | Association given | |

TABLE 16 DESCRIPTION OF DATASET FUJITA ET AL. 2013

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Fujita *et al.* (2013) | |
| | | |
| Country | Netherlands | |
| Ecosystem/vegetation | Grassland, heath | |
| Period | 2011 | |
| Soil type | Different soil types | |
| Amount of locations | 36 | |
| Sample depth | 0-15 cm | |
| | | |
| Duplicates | 3 subsamples, mixed to one | |
| Soil Parameters | Soil contents (solid phase) | C, N, P (mineral) |
| | Chloroform fumigation extraction | C, N (microbe) |
| | KCl extraction | N-NH4, N-NO3, pH |
| | Olsen extraction | P-PO4, |
| | Oxalate extraction | P, Al, Fe |
| | Soil texture | |
| | Bulk density | |
| | Net mineralization rates (incubation experiment) | |
| Carbon and Nutrient pools | | C, N, P |
| Vegetation parameters | Nutrient content (N, P) in above-ground biomass | |
| Species composition | Cover of vascular plant species | |

TABLE 17. DESCRIPTION OF DATASET ORDONEZ ET AL. 2010

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Ordonez et al. 2010 | |
| | | |
| Country | Netherlands | |
| Ecosystem/vegetation | Grassland, shrubs, forests | |
| Period | 2009? | |
| Soil type | Different soil types | |
| Amount of locations | 51 | |
| Sample depth | 0-15 cm | |
| | | |
| Duplicates | 5 subsamples, mixed to one | |
| Soil Parameters | Soil contents (solid phase) | C, N, P (mineral) |
| | KCl extraction | N-NH4, N-NO3, pH |
| | Olsen extraction | P-PO4, |
| | Net mineralization rates (incubation experiment) | |
| Carbon and Nutrient pools | | C, N, P |
| Vegetation parameters | Nutrient content (N, P) in plant leaves | |
| Species composition | Cover of vascular plant species | |

TABLE 18. DESCRIPTION OF DATASET OLDE VENTERINK ET AL. 2002

| **Monitoring Characteristics** | **Type of measurement** | **Elements included** |
|---|---|---|
| Reference | Olde Venterink *et al.* (2002) | |
| Country | Netherlands, Belgium | |
| Ecosystem/vegetation | Grasslands | |
| Period | 1995 - 2003 | |
| Soil type | Different soil types | |
| Amount of locations | 47 | |
| Sample depth | 0-10 cm | |
| Duplicates | No duplicate | |
| Soil Parameters | Soil contents (solid phase) | N, P (mineral), SOM |
| | KCl extraction | N-NH4, N-NO3, pH |
| | ALA extraction | P-PO4 |
| | Net mineralization rates (incubation experiment) | |
| Carbon and Nutrient pools | | N, P |
| Vegetation parameters | Nutrient content (N, P) in above-ground biomass | |
| Species composition | Cover of vascular plant species | |

* Permission of the authors is required to use this dataset.

# Appendix III Available dataset for model validation

TABLE 19 DESCRIPTION OF DATASET SPEULD

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Van der Salm *et al.* (1998) | |
| Location | Speulderbos | |
| Ecosystem/vegetation | Forest, Douglas fir | |
| Area | | |
| Amount of replicates | | |
| Period | 1990-1995 | |
| Frequency | e.g. monthly or weekly | |
| Soil Parameters (frequency) | Soil type | |
| | Bulk density | |
| | CEC | |
| Carbon and Nutrient pools | | |
| Soil moisture | Lysimeter cups (bi-weekly) | pH, NH4, NO3, Cl, Na, K, Al, Ca, Mg, Fe, Mn, P, S, Si, Zn |
| Vegetation parameters | Biomass fitted to growth data | |
| | Nutrient contents: no | |
| Species composition | No | |
| Meteo data | e.g. Rainfall, temperature | |
| Hydrology | Modelled by SWATRE | |
| Deposition | Measured bi-weekly | |

TABLE 20 DESCRIPTION OF DATASET RISDALSHEIA

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Mol-Dijkstra and Kros (2001) | |
| Location | Risdalheia | |
| Ecosystem/vegetation | Pine and birch with heather | |
| Area | | |
| Amount of replicates | | |
| Period | 1984-1997 | |
| Frequency | | |
| Soil Parameters (frequency) | Soil type | |

| | | |
|---|---|---|
| | Bulk density | |
| | Porosity | |
| | CEC | |
| | SO4 adsorption | |
| | Organic matter | |
| Carbon and Nutrient pools | | |
| Mineralisation | Measured in 1994-1996 | |
| Nitrification | Measured in 1994-1996 | |
| Soil moisture | Concentrations (several per year) | pH, NH4, NO3, Cl, Na, K, Al, Ca, Mg, Fe, Mn, P, $SO_4$ |
| Vegetation parameters | Litter fall | |
| | Nutrient contents | N, K, Ca, Mg |
| Species composition | | |
| Meteo data | Rainfall, temperature | |
| Hydrology | Modelled by SWATRE | |
| Deposition | Measured yearly (we only have yearly data) | |

TABLE 21 DESCRIPTION OF DATASET SPEULD

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Grobben et al. (unpublished data)<br>(Kemmers, 1999; Kemmers *et al.*, 2000) | |
| Location | 7 sites | |
| Ecosystem/vegetation | Wet grassland | |
| Area | | |
| Amount of replicates | | |
| Period | 1999 | |
| Frequency | | |
| Soil Parameters (frequency) | Soil type | |
| | Bulk density | |
| | CEC | |
| Carbon and Nutrient pools | | |
| Soil moisture | Lysimeter cups (monthly) | pH, Na, K, Ca, Mg, Fe, $SO_4$, Cl, $NH_4$, $NO_3$ |
| Vegetation parameters | Biomass:No | |
| | Nutrient contents: no | |
| Species composition | No | |
| Meteo data | e.g. Rainfall, temperature | From closest KNMI station |
| Hydrology | Modelled by SWATRE | |

| | | |
|---|---|---|
| Deposition | Taken from modelled maps by RIVM | |

TABLE 22 DESCRIPTION OF DATASET VEENKAMPEN

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Mol et al, (unpublished data) | |
| Location | Wageningen | |
| Ecosystem/vegetation | Wet grassland | |
| Area | | |
| Amount of replicates | | |
| Period | 1983-2006 | |
| Frequency | | |
| Soil Parameters (frequency) | Soil type<br>Bulk density<br>CEC | |
| Carbon and Nutrient pools | ‘86, ‘87, ‘91, ‘93, ‘97 | C, N, P, K |
| Soil moisture | 1993, 2002, 2006 | pH, Na, K, Ca, Mg, Fe, $SO_4$, Cl, $NH_4$, $NO_3$ |
| Vegetation parameters | Biomass: 1983-1990, 2006<br>Nutrient contents: 1983-1990, 2006 | N, P, K |
| Species composition | ? | |
| Meteo data | e.g. Rainfall, temperature | From closest KNMI station |
| Hydrology | | |
| Deposition | Taken from modelled maps by RIVM | |

TABLE 23 DESCRIPTION OF DATASET HULSHORSTERZAND

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Wamelink *et al.* (2001) | |
| Location | Hulshorsterzand | |
| Ecosystem/vegetation | 4 stages (bare soil to forest) | |
| Area | | |
| Amount of replicates | | |
| Period | 1993-1994 | |
| Frequency | | |
| Soil Parameters (frequency) | Soil type<br>Soil moisture<br>CEC<br>pH<br>Soil moisture<br>N mineralisation | |

| | | |
|---|---|---|
| Carbon and Nutrient pools | 1994 | C, N |
| Soil moisture | No | |
| Vegetation parameters | Biomass: 1994 | |
| Species composition | Yes | |
| Meteo data | Rainfall yearly | From closest KNMI station |
| Hydrology | | |
| Deposition | Taken from modelled maps by RIVM | |

TABLE 24 DESCRIPTION OF DATASET SELLINGEN

| Monitoring Characteristics | Type of measurement | Elements included |
|---|---|---|
| Reference | Wamelink et al, 2001 | |
| Location | Sellingen | |
| Ecosystem/vegetation | 4 stages Oak forest | |
| Area | | |
| Amount of replicates | | |
| Period | 1999 | |
| Frequency | | |
| Soil Parameters (frequency) | Soil type | |
| | Bulk density | |
| | CEC | |
| Carbon and Nutrient pools | 1999 | C, N |
| Soil moisture | 1996 | pH, Na, K, Ca, Mg, Fe, $SO_4$, Cl, $NH_4$, $NO_3$ |
| Vegetation parameters | Biomass: 1999 | |
| | Nutrient contents: 1999 | N, K, Ca, Mg |
| Species composition | No | |
| Meteo data | e.g. Rainfall, temperature | Same as Hulshorsterzand |
| Hydrology | | |
| Deposition | Taken from modelled maps by RIVM | |

## Datasets

**Meteo** (resolution = 1 hour)

- solar radiation
- net radiation
- wet bulb T
- dry bulb T
- wind speed
- wind direction
- rainfall
- albedo (sky)
- albedo(ground)
- soil T at 10 cm
- soil T at 30 cm
- nr. of minutes that the surface is wet
- soil moisture (theta probe)

**Precipitation chemistry (resolution = weekly)**

- pH
- conductivity
- alkalinity
- Na, K, Ca, Mg, Fe, Al, PO4-P, NOx-N, NH3-N, Cl, SO4-S, DOC, Total-N

**Soil solution (two depths (which?), six samples per depth and sampling event, every two weeks)**

- pH
- conductivity
- alkalinity
- Na, K, Ca, Mg, Fe, Al, PO4-P, NOx-N, NH3-N, Cl, SO4-S, DOC, Total-N

**Vegetation surveys (2m × 2m plots for non-woodlands, 10m × 10m for woodlands)**

- plant species occurrence for approx. 100 plots

### **Site descriptions of the** ECN sites

Alice Holt

The history of Alice Holt forest can be traced back over 2000 years and is believed to have originated during the Atlantic period. Iron Age and Roman relics found within the forest point to a long history of human inhabitation. The forest has belonged to the crown since William the Conqueror adopted it as a Royal Hunting Forest. The Forestry Commission has actively managed the forest since 1924 and it has been the focus of research activities since 1946.

Alice Holt Forest Park covers 851 hectares of mainly Corsican pine but approximately 140 ha. of original 1820 oak still remain. The ancient forest is now a truly multi-purpose woodland where research, conservation, timber production and recreation co-exist.

| | |
|---|---|
| Min Altitude | 110 m |
| Max Altitude | 125 m |
| Area of Site | 850 ha |
| Mean annual temperature* | 10.7 °C |
| Mean annual rainfall* | 850 mm |

### Cairngorms

The Cairngorms site, which joined the ECN network in summer 1999, is located high in the Cairngorms, near Aviemore in Speyside. The site lies on the western flank of the Cairngorms and is the catchment of the Allt a' Mharcaidh (a site in the ECN freshwater network). It is part of the Invereshie and Inshriach National Nature Reserve, within the Cairngorms National Park, and covers some 10 km2. The site is supported by a consortium of Scottish Natural Heritage (SNH), the Natural Environment Research Council (through the Centre for Ecology and Hydrology) and The James Hutton Institute (JHI). ECN monitoring at the site is co-ordinated by CEH.

ECN Cairngorms is also part of the UK's first Long-Term Socio-Ecological Research platform, the Cairngorms National Park.

This site is in the UK's sub-arctic zone and is an important link not only to other upland ECN sites but to sites in the Alps and Pyrenees (GLORIA network) and also to networks in the Arctic (SCANNET network and INTERACT project).

| | |
|---|---|
| Min Altitude | 320 m |
| Max Altitude | 1110 m |
| Area of Site | 1000 ha |
| Mean annual temperature* | 4.7 °C |
| Mean annual rainfall* | 872 mm |

### Drayton

A heavy clayland site, representative of 2 million hectares of similar soils in lowland England, where agricultural experiments have been conducted for 50 years. The farm system is based on autumn sown combinable crops and grassland. Hedges and ditches contribute to biological diversity.

| | |
|---|---|
| Min Altitude | 40 m |
| Max Altitude | 80 m |
| Area of Site | 190 ha |
| Mean annual temperature* | 10.3 °C |
| Mean annual rainfall* | 630 mm |

### Hillsborough

A lowland grassland site situated at the Agri-Food and Biosciences Institute, Co. Down, Northern Ireland and representative of grassland in much of the north-western United Kingdom. There are several long-term experiments, for example on slurry application and nitrogen cycling on grazed plots receiving different levels of nitrogen input. A large part of the site used for the biological aspects of ECN monitoring is estate woodland (Hillsborough Forest) consisting of mature mixed woodland and conifer plantation. Many of the vegetation plots are located within this forested area, as are sections of the butterfly, carabid beetle, spider and bird transects.

| | |
|---|---|
| Min Altitude | 110 m |
| Max Altitude | 170 m |
| Area of Site | 400 ha |
| Mean annual temperature* | 9.2 °C |
| Mean annual rainfall* | 1116 mm |

Moor House

This site lies in the North Pennine uplands of England. It is England's highest and largest terrestrial National Nature Reserve (NNR). Habitats include exposed summits, blanket peatlands, upland grasslands, pastures, hay meadows and deciduous woodland. A large part of the catchment of the River Tees, from its source near Great Dun Fell to High Force waterfall, is included in the reserve. The Trout Beck, which has its catchment entirely within the Moor House National Nature Reserve, is an ECN Freshwater Site

| | |
|---|---|
| Min Altitude | 290 m |
| Max Altitude | 848 m |
| Area of Site | 7500 ha |
| Mean annual temperature* | 5.8 °C |
| Mean annual rainfall* | 2044 mm |

North Wyke

A lowland grassland site typical of conditions in wetter, western Britain, with predominately impermeable clays of the Culm Measures. Current research at North Wyke is helping to address some of agriculture’s most pressing challenges, for example mitigating and adapting to climate change, protecting natural resources and sustaining the rural economy in grassland dominated regions.

| | |
|---|---|
| Min Altitude | 120 m |
| Max Altitude | 180 m |
| Area of Site | 250 ha |
| Mean annual temperature* | 9.9 °C |
| Mean annual rainfall* | 1063 mm |

Porton

As well as being a Site of Special Scientific Interest (SSSI), Porton Down is also a Special Area of Conservation (SAC) and a Special Protection Area (SPA) covering over 1500 hectares. It constitutes the largest uninterrupted tract of semi-natural chalk grassland in Britain, a habitat which has declined by more than 80% in the last 50 years. As well as the grassland the site supports large areas of mixed scrub, including juniper, and broadleaved, mixed and coniferous woodland.

| | |
|---|---|
| Min Altitude | m |
| Max Altitude | m |
| Area of Site | 1227 ha |
| Mean annual temperature* | 9.7 °C |
| Mean annual rainfall* | 803 mm |

Rothamsted

The oldest continually functioning agricultural research station in the world. The 'Classical Experiments', started between 1843 and 1856, plus wilderness sites, have been used by successive generations of scientists and continue to form a unique resource for studying environmental change.

| | |
|---|---|
| Min Altitude | 94 m |

| | |
|---|---|
| Max Altitude | 134 m |
| Area of Site | 330 ha |
| Mean annual temperature* | 10.1 °C |
| Mean annual rainfall* | 692 mm |

Snowdon

Yr Wyddfa/Snowdon is an upland ECN site incorporating the summit of Yr Wyddfa or Snowdon, the highest mountain in England and Wales, 19km south-east of Bangor in North Wales. It is co-located with the Nant Teyrn freshwater site. The dominant vegetation is acidic grassland with Festuca ovina (sheep's fescue) and Agrostis species (bent grass) in the drier areas and Nardus stricta (mat grass) in the wetter areas. The site is part of the Yr Wyddfa/Snowdon National Nature Reserve, managed by Natural Resources Wales (NRW) under agreement with the owner. The land is unenclosed and grazed by sheep and a small herd of feral goats.

| | |
|---|---|
| Min Altitude | 298 m |
| Max Altitude | 1085 m |
| Area of Site | 700 ha |
| Mean annual temperature* | 7.4 °C |
| Mean annual rainfall* | 3784 mm |

Sourhope

The ECN site at Sourhope lies 15 miles south-east of Kelso near the head of the Bowmont valley on the western slopes of the Cheviot. The site covers an area of approximately 1100 hectares. The vegetation at the Target Sampling Site is representative of that across both the farm and many parts of the uplands in southern Scotland consisting of coarse grassland dominated by White bent (Nardus stricta) and Flying bent (Molinia caerulea). The site is relatively exposed and access can be difficult due to prolonged snow cover during the winter months.

| | |
|---|---|
| Min Altitude | 200 m |
| Max Altitude | 601 m |
| Area of Site | 1119 ha |
| Mean annual temperature* | 7.4 °C |
| Mean annual rainfall* | 971 mm |

Wytham

Wytham is 5 km north west of Oxford. About half the site is woodland, the rest organic mixed farmland. Roughly a third of the wooded area is ancient woodland which, to our knowledge, has never been cleared and there has been continuity of tree cover since the prehistoric 'wild wood'. It has however had a long history of management, which for many hundreds of years took the form of coppicing. Within the woodland there are patches of semi-natural grassland, of both ancient and recent origin, and scrub.

| | |
|---|---|
| Min Altitude | 60 m |
| Max Altitude | 165 m |
| Area of Site | 770 ha |
| Mean annual temperature* | 9.9 °C |
| Mean annual rainfall* | 750 mm |