Technical documentation of the soil model VSD+

Status A

J.P. Mol-Dijkstra & G.J Reinds

WOt-technical report 88

WAGENINGEN
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This document contributes to the body of knowledge which will be incorporated in more policy-oriented publications such as the National Nature Outlook and Environmental Balance reports, and thematic assessments.

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Abstract

Mol-Dijkstra, J.P.& G.J Reinds (2017). *Technical documentation of the soil model VSD+; Status A.* Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu), WOt-technical report 88. 88 p.; 9 Figs; 11 Tabs; 21 Refs; 7 Annexes.

VSD+ is a model to calculate effects of atmospheric deposition and climate change on soil acidification, nutrient availability and carbon sequestration. The model has been developed to support emission abatement strategies of sulphur (S) and nitrogen (N) in Europe. This document contains a summary of the model theory, technical documentation and descriptions of testing, validations and the sensitivity analysis of the model. The processes described in the paper about VSD+ have been tested successfully. The sensitivity analysis showed that the constant for the equilibrium between H^+ and Al^{3+} in the soil solution and the weathering rate of Ca are the parameters that to a large extent determine the value of the simulated pH. For base saturation, most important parameters are the exchange constant between H^+ and base cations and the weathering of Ca. For the C/N ratio of soil organic matter, litterfall of C and N and the uptake of N are important influencing factors. The nitrate concentration strongly depends on the leaching flux and the net N input.

Keywords: VSD+ model, soil acidification, soil nutrient availability, carbon sequestration, atmospheric deposition, climate change

Referaat

Mol-Dijkstra, J.P. & G.J Reinds (2017). *Technische documentatie van het VSD+ model; Status A.* Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu), WOt-technical report 88. 88 blz.; 9 fig.; 11 tab.; 21 ref; 7 Bijlagen.

VSD+ is een model om de gevolgen te berekenen van atmosferische depositie en klimaatverandering voor bodemverzuring, de beschikbaarheid van voedingsstoffen en het vastleggen van koolstof. Het model is ontwikkeld ter onderbouwing van strategieën om de uitstoot van zwavel (S) en stikstof (N) in Europa te verminderen. Dit document biedt een samenvatting van de theorie waar het model op gestoeld is, de technische documentatie hiervan alsmede een beschrijving van het testen, het valideren en de sensitiviteits-analyse van het model. De processen zoals beschreven in het artikel over VSD+ zijn met goed gevolg getest. De gevoeligheidsanalyse gaf aan dat de constante voor het evenwicht tussen H^+ en Al^{3+} in de bodem-oplossing en de Ca-verweringssnelheid de parameters zijn, die voor een groot gedeelte de waarde van de gesimuleerde pH bepalen. Voor basenverzadiging zijn de belangrijkste parameters de uitwisselingsconstante tussen H^+ en basische kationen en de verwering van Ca. Voor de C/N ratio van bodemorganische stof zijn C en N in het strooisel en de opname van N zeer bepalende factoren. De nitraatconcentratie hangt sterk samen met het nerslagoverschot en de netto input van N.

Trefwoorden: VSD+ model, bodemverzuring, beschikbaarheid van nutriënten, koolstofvastlegging, atmosferische depositie, klimaatverandering

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Preface

This technical document gives an overview of the documentation to obtain the quality level A for the VSD+ model. Gathering this information forced us to review the model critically, which for instance led to some corrections in the model description.

We like to thank Max Posch for his contribution to the testing of the model and documentation of 'Monitor' and the auditors Janien van der Greft, Geerten Hengeveld and George van Voorn for their critical reviews.

Janet Mol and Gert Jan Reinds

Contents

Summary

VSD+ is a model developed to calculate effects of atmospheric deposition and climate change on soil acidification, nutrient availability and carbon sequestration. Simulated values for pH and nitrogen such as C/N ratio and nitrate concentration can be used in models that predict occurrence probabilities of plant species as a function of abiotic conditions. VSD+ was developed to support the emissions abatement of S and N in Europe and is also used to calculate critical loads for nitrogen and sulphur in support of Dutch environmental policies. The Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu) has the policy that all models that are used in WOT context must have the quality status A, which means that the model is described technically, has been tested, validated and a sensitivity analysis has been performed. This information is gathered in this report.

This document contains a summary of the model theory, a technical documentation and descriptions of testing, validation and a sensitivity analysis of the model. The processes described in the paper about VSD+ have been tested successfully. A sensitivity analysis showed that the constant for the equilibrium between H^+ and Al^{3+} in the soil solution and the weathering rate of Ca are the parameters for pH. For base saturation, most important parameters are the exchange constant between H^+ and Bc and the weathering of Ca. For C/N ratio litterfall of C and N and the uptake of N are important influencing factors. The simulated nitrate concentration strongly depends on the leaching flux and the net N input.

1 Introduction

As a result of the relationship between air pollution and acidification of soils and waters that was observed in the late 1970s, the United Nations Economic Commission for Europe (UNECE) initiated the Convention on Long-range Transboundary Air Pollution (LRTAP). Under this convention a number of working groups were established, to investigate all relevant aspects of air pollution and its effects on ecosystems, crops, human health and materials (Bull *et al.*, 2001). One of this working groups is the ICP on Modelling and Mapping (ICP M&M) which is responsible for the assessment of regional critical loads for Europe. Critical loads are the maximum tolerable inputs of sulphur (S) and nitrogen (N) that, on an infinite time scale and according to current knowledge, will not lead to significant harmful effects on the ecosystem (Nilsson and Grennfelt, 1988). Critical loads can be used to determine where ecosystems are threatened by atmospheric deposition, by comparing the critical load with the present deposition. This information on critical load exceedances is used to establish cost effective abatement strategies for S and N, by targeting these reductions in such a way that exceedances are minimized at minimum abatement costs (e.g. Gregor *et al.*, 2001, Amann *et al.*, 2007). Critical loads for acidity are commonly modelled with a simple mass balance (SMB) model (Sverdrup and De Vries, 1994). Critical loads for nutrient nitrogen can be computed with SMB as well, but have also been derived from N addition experiments in the field (empirical critical loads).

Although critical loads give the maximum allowable deposition that, on an infinite time scale, protects an ecosystem, it does not provide information on the time development of pollution induced stress and its effects on the ecosystem. Furthermore, if a critical load is currently exceeded (or was exceeded in the past), neither the critical load nor its excess can be used to estimate the time delay before a criterion, i.e. the critical value of a geochemical indicator associated to a biological effect, is violated. Nor can one estimate from the critical load the time delay to geochemical recovery if deposition is reduced to or below the critical load (Posch *et al.*, 2003). Therefore, interest shifted from critical loads alone towards the use of dynamic acidification models for soils and surface waters, that are capable of simulating the change in time of the chemical ecosystem status as a function of changing deposition (Grennfelt *et al.*, 2001; Posch *et al.*, 2003). To have a model that is fully compatible with critical loads, the VSD model was developed (Posch and Reinds, 2009) that extends the SMB model by incorporating cation exchange and time-dependent N immobilization. The VSD model requires a minimum set of input data and is designed for application on the European and continental scale. It is capable of simulating the effects of critical load exceedances in terms of time delays to 'damage' and, in the case of sufficient deposition reduction, to 'recovery' and can be also used to set deposition targets for the short to medium term, called target loads.

With the strong reductions in sulphur emissions that have been achieved in Europe over the last decades, the role of nitrogen deposition on terrestrial ecosystems has become more important. More insight is now required in how nitrogen effects for example vegetation composition. The VSD model, however, has a very simple way of modelling N as it does not include process descriptions for nutrient cycling. Therefore the VSD model was extended with a sub-model, RothC, that models the dynamics of carbon and nitrogen in the soil as a function of C and N inputs and soil characteristics. This VSD+ model (Bonten *et al.*, 2016) is thus much better suited to be linked to vegetation models that compute plant species occurrence probabilities as a function of pH and N characteristics in soils.

The Statutory Research Tasks Unit for Nature & the Environment has the policy that all models, that are used for their tasks, have a defined quality level A (see Annex 7). This means that the models are well documented and tested. In this report we document the VSD+ model. In Chapter 2, the theory is described. The technical documentation can be found in Chapter 3, followed by the users documentation in Chapter 4. The testing of the model is described in Chapter 5, calibration and validation in Chapter 6. Chapter 7 handles about the sensitivity analyses of VSD+.

2 Theory

The theory of the model is described in two peer reviewed papers: one about VSD (Posch and Reinds, 2009; section 1 and 2) that describes all chemical processes such as cation exchange, leaching etc, and one about VSD+ (Bonten *et al.*, 2016; section 1 and 2.1) that describes the nutrient cycling that is modelled in VSD+.

2.1 Purpose and application area

The purpose of the model is described in the introduction for VSD by Posch and Reinds (2009). The model is intended to simulate acidification and eutrophication of the soil in response to atmospheric deposition. Many models with the same purpose are so called 'research models ', which are too detailed to be able to be applied on national or European scale. VSD is a simple model that requires little detailed input and therefore suitable for regional to continental scale. Quote from Posch and Reinds (2009): "*Here we describe the ' very simple dynamic (VSD) model ', which is designed for sites with few dates available and applications on a large regional or continental scale.*" In applications on regional to European scale, spatial information like soil type and vegetation type and climate is required. This spatial information is gridded to cells. A regional model application consists of applying the model (as a point model) to each grid cell or, for larger grid cells, to each sub cell where that is homogenous with respect to soil, vegetation and climate characteristics.

VSD + is an extension of VSD with the carbon (C) and nitrogen (N) cycle included. This was required because, due to the decrease of the emission and deposition of sulphur (S), the focus of the policy and research has shifted to biodiversity and nitrogen (Baker *et al.* (2016)). The extra purpose of VSD+ is to simulate the effect of atmospheric deposition on acidity and nitrogen parameters that can influence the occurrence probability of plant species.

Posch and Reinds (2009; section 2), state that the model was developed for the calculation of soil acidification on non-calcareous soils, but VSD+ is also applicable on calcareous soils. It is not designed for wet ecosystems. In section 4 of Bonten *et al.* (2016) it is described that the model is not extensively tested on heathland and grassland, but that it is suitable for this vegetation type under dry conditions, since the soil processes in such ecosystems are similar to those in forests. For wet circumstances, the model would require the simulation of processes that take place under low-oxygen conditions such as reduction and oxidation.

2.2 Simplifications

De Vries *et al.* (1989) describe in section 2 of their paper some key assumptions and simplifications made in the design of the SMART model, a forerunner of VSD. The same considerations were taken for VSD and VSD +. Posch and Reinds (2009) describe the assumptions for VSD in section 2 of their paper. The VSD model is the simplest extension of the steady-state SMB model into a dynamic model by including cation exchange and time-dependent N immobilisation (accumulation). Therefore, many simplifications can be found in the description of the simple mass balance (SMB) model (UBA, 2004; section 5.3). Simplifications in the N-balance, described in UBA (2004; section5.3.1) concern neglecting NH_4-adsorption by clay minerals, loss of N due to fire, erosion and volatilisation. In contrast to SMB, N fixation and NH_4 leaching is not neglected in VSD+. So, the assumptions about neglecting N-fixation and NH_4 leaching do not apply to VSD+. Simplifications in calculation of acidity are described in UBA (2004; section 5.3.2).

The main difference between VSD and VSD + is the addition of the C-and N-cycle and organic matter dynamics by inclusion of the model of RothC-26.3 (Coleman and Jenkinson, 2014). Bonten *et al.* (2016) have chosen to include RothC-26.3 as the model for C and N dynamics, because that model performs well and because it is simple and needs a few inputs which are easily obtainable (see part 1 in Coleman and Jenkinson (2014).

3 Technical documentation

3.1 Meta-information

Part of the meta-information is given by Bonten *et al.* (2016). The complete information is given in Table 1.

Table 1
Meta-information VSD+

Name software	VSD+
Developers	Luc Bonten, Gert Jan Reinds, Maximilian Posch
Version	VSD+ 1.4, Studio versie 5.5.1
Releasedate	10 Juni 2016
Purpose	VSD+ calculates soil acidification, nitrogen availability and carbon sequestration in response to atmospheric deposition and climate change
Knowledge	The user needs some soil chemical or ecological knowledge to apply this model
Scale	Point to continental scale. Time steps of one year
Input	Model input concerns ecosystem inputs like deposition and litter fall, precipitation excess, state variables like base saturation and C/N ratio and soil physical and chemical parameters.
Output	See user documentation. Model outputs concern amounts of Ca, Mg, K, Al, and H at the exchange complex, the five organic matter pools, N fluxes like mineralisation, leaching, (de)nitrification and the concentrations of all considered elements in soil solution
Communication with user	Graphical user interface called VSD+ studio
Operating system	Windows XP and higher
Program language	Intel Visual Fortran (GUI: Embarcadero C++ Builder)
Availability	Download from http://wge-cce.org/Methods_Models/Available_Models
Costs	Free
Contact adress	Wageningen Environmental Research (WEnR) P.O. Box 47, 6700AA Wageningen, The Netherlands
Contact person	Gert Jan Reinds (gertjan.reinds@wur.nl)
Disclaimer	WEnR is not responsible nor are the model makers for any (financial) damage that the model may cause in any way

3.2 Program structure

3.2.1 VSD+ forward calculation

The program structure is shown schematically in Figure 1. The main program is called runVSDp, which calls subroutines which are included in several dll's, marked by different colours in Figure 1. Within runVSDp, first the input is read via the subroutine VSDpin (1). Within VSDpin, first the input is read that is equal to the input for VSD, in the subroutine Readinp (1.1). Then the additional input for VSDp is read in the subroutine readinpVSDp (1.2) and finally, a number of input parameters is converted in the subroutine VSDprep (1.3) ; see CCE (2001)

After reading the input, the subroutine VSDprun is called (2), in which the simulations of the soil processes and nutrient cycling take place. First, if desired, per time step adjustment is made for a sea

salt SO_4 in the subroutine seasalts (2.1) by correcting the SO_4 input (see UBA, 2004, Chapter 2). Then, each time step VSDp is called (2.2). Two subroutines are called within VSDp, first CNorg, in which the decomposition of organic matter in different compartments is calculated as described in Bonten *et al.* (2016) (2.2.1), then the net fluxes of all elements in VSDp are calculated, and then VSDcore is called (2.2.2), for which the chemical equations are described by Posch and Reinds (2009). This is the subroutine in which the concentrations in the soil moisture are calculated and this subroutine is also present in VSD. In VSDprun all output per time step is saved. Finally, monitor is called, which produces the graphic display of the output (3).

All subroutines, except monitor, contain a header with the description of the purpose of the subroutines and their interfaces (see Annex 1). The interface of monitor is described in Annex 2.

The source code is provided with comments, so that the code can easily be understood by someone who knows the Fortran programming language.

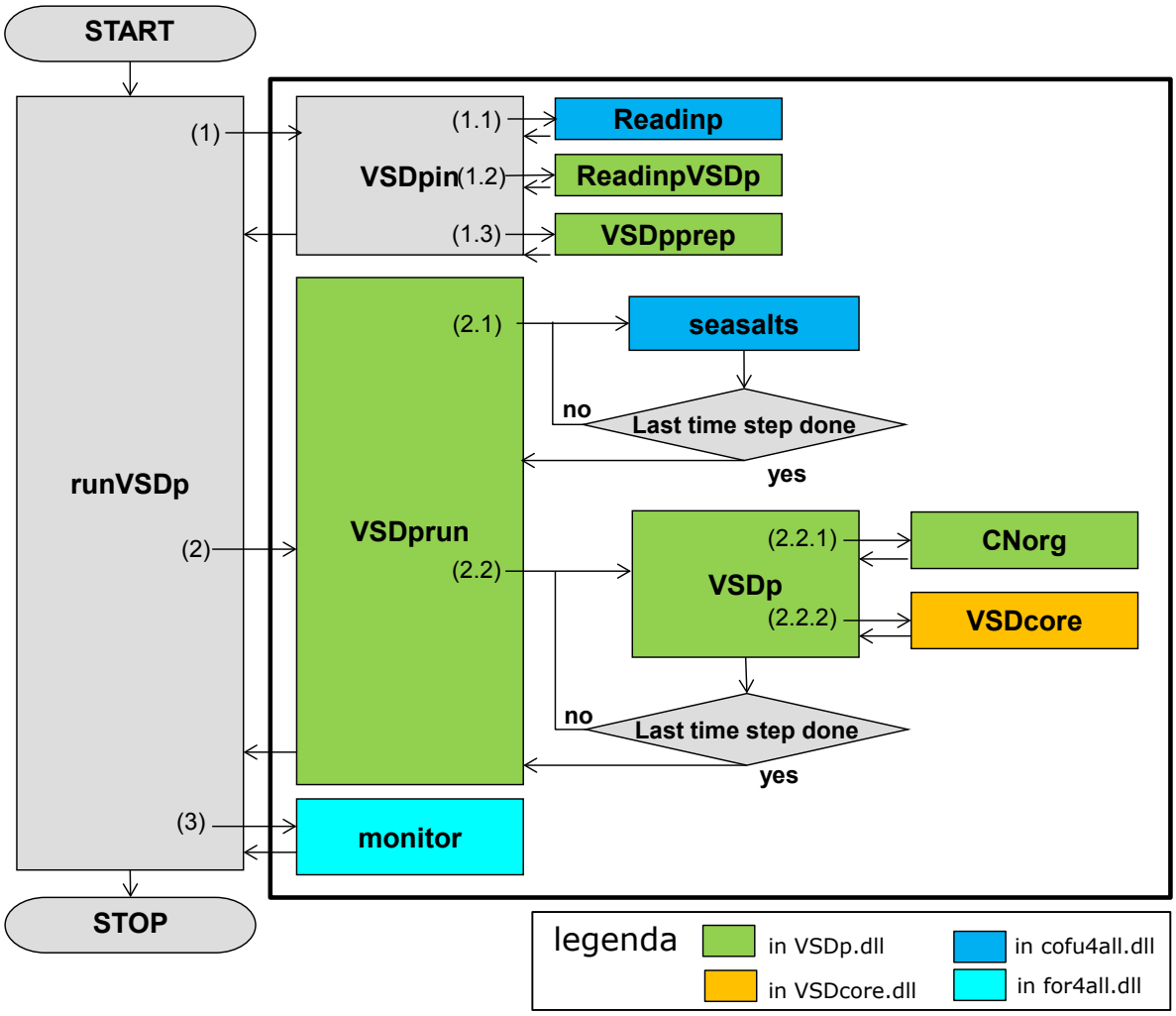

Figure 1 *Flowchart VSD+ for forward calculation*

3.2.2 Critical load calculation

A single site calculation of critical loads is done in the graphical user interface (GUI). First, the same input is read (step 1) as described in section 3.2.1 and then the critical loads (CL) are calculated (step 2) in the subroutine VSDpSMB (Figure 2), which is included in VSDp.dll. The header of VSDpSMB.f90 is shown in Annex 1. The theory behind the calculations and the equations are given in the help-file under 'Steady state calculations', the last item under VSD+ model. Supplementary input is required about the criterion on which the critical load is based (e.g. critical pH, critical Al/Bc ratio etc.). This information must be specified in the GUI.

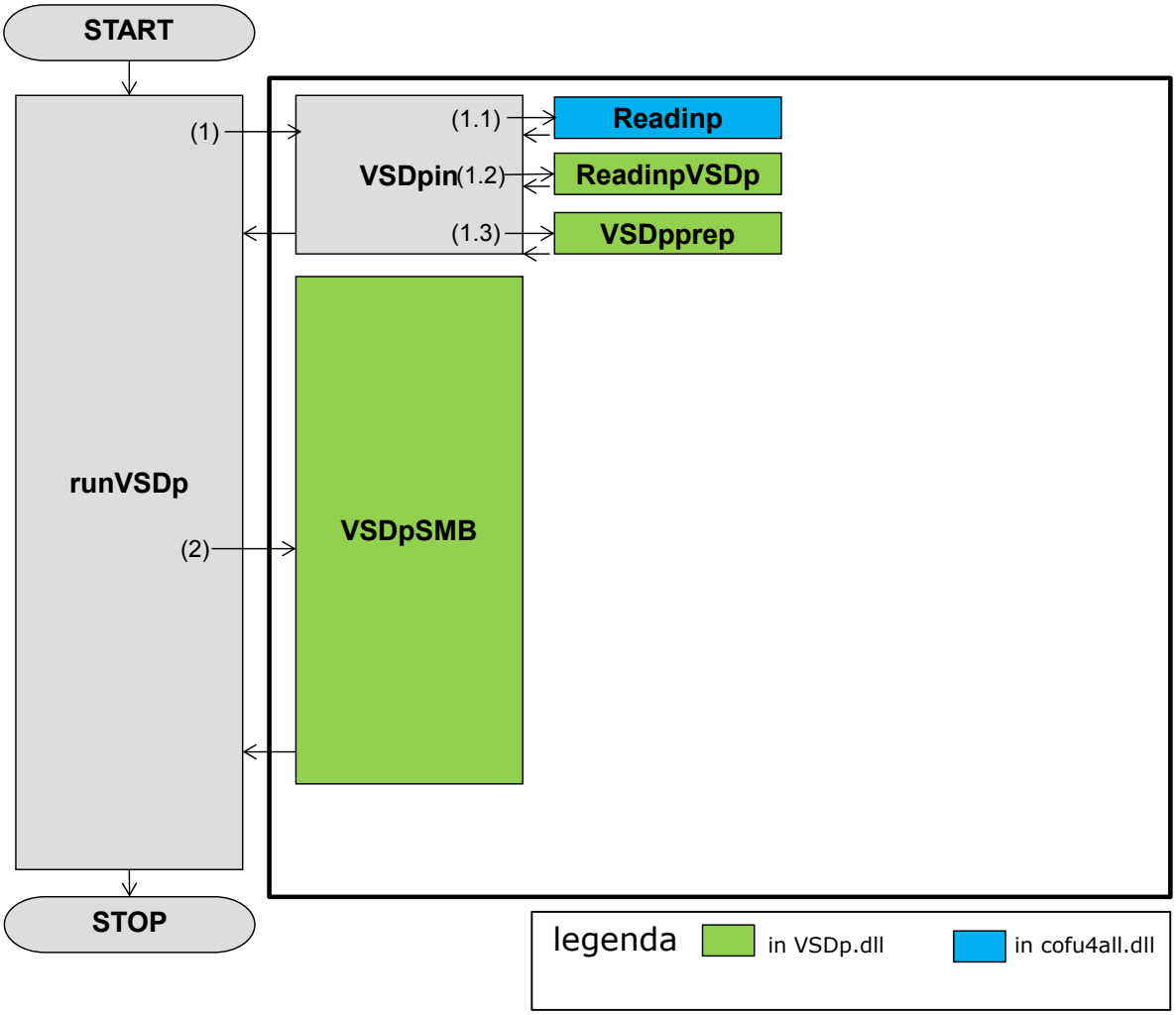

Figure 2 *Flowchart VSD+ for critical load calculations*

3.3 VSDpStudio: a description how the GUI connects to the VSD+ model

3.3.1 Introduction

For ease of use of the VSD+ model, a graphical user interface (GUI) was developed called VSDpStudio (Bonten *et al.*, 2016). This GUI facilitates the creation and change of input files, running of the model, comparing results from different runs and creation of output files and graphs. In this chapter we describe how this GUI interacts with the VSD+ model. The GUI can be used as an alternative for the command line tool runVSDp that was shown described in section 3.2.1.

3.3.2 Method

VSDpStudio was programmed in C++ using Embarcadero C++ Builder 2010. It interacts with the VSD+ model through interfaces with the VSD+ dll and it's auxiliary dlls (Figure 3).

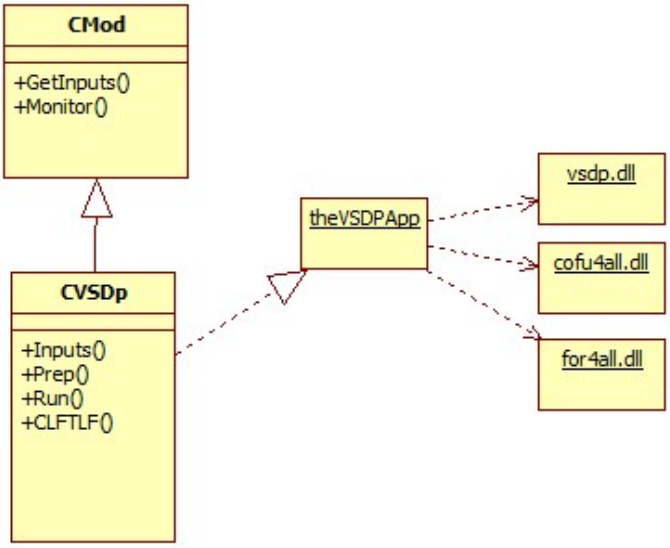

Figure 3 *Schematic overview of interfaces between VSDpStudio and the VSD+ model*

In C++ a base class was defined for the soil acidification models at Wageningen Environmental Research (WEnR) (notably SMART, VSD and VSD+) called CMod. This class contains functions that are common to these models such as the reading of an input file with parameters (GetInputs) and the construction of graphs with simulation results for an encapsulated postscript file (Monitor). For VSD+ a derived class was made CVSDp, that builds on the base class with VSD+ specific code. The function Inputs calls the base function GetInputs for most of the input parameters, but also calls VSD+ specific routines for input parameters specific for VSD+. The function Prep prepares the input parameters for use in the model core, by e.g. conversion of exchange constants to the proper units and construction of input time series. The function Run runs the VSD+ model. The function CLFTLF computes critical loads. In VSDpStudio an object is constructed from the class CVSDp: VSDpApp. This object loads the dll's it needs for reading in an input file, converting the input, running the model and producing output. All these tasks have been programmed in the Fortran VSD+ routines and exported to the dll's. These dll's, in turn, are used by VSDpStudio, so that we are sure that the way inputs are read, the model is run and output is produced is identical to the way the command line Fortran version of VSD+ does (provided that the same values for the inputs to these routines are used).

In Table 2 an overview is provided of the main functions and dll's used by the various functions in VSDpStudio.

Table 2

Most important Fortran functions used by VSDpStudio and their purpose

C++ function	dll	Fortran subroutine	Purpose
GetInputs	cofu4all	readinp	read input
Inputs	vsdp.dll	readinpvsdp	read vsd+ specific parameters
Inputs	vsdp.dll	readinpagro	read vsd+ parameter for agricultural soils
Prep	vsdp.dll	vsdpprep	prepare the inputs
Run	vsdp.dll	vsdprun	run the model
Monitor	for4all.dll	monplot	plot graphs with simulation results
Monitor	for4all.dll	monwrite	write simulation results to ascii file
CLFTLF	vsdp.dll	vsdpsmb	compute critical loads

Apart from the functions given in Table 2**,** a number of auxiliary Fortran function are used to e.g. correct critical loads for seasalts, read in observation files etc.

To facilitate the interface between C++ and Fortran, a simple tool was developed to extract the function and subroutine interfaces from the Fortran source codes and convert these into a C++ interface to be used in VSDpStudio (*extrcall.f90*). As an example of how such an interface is created, we use here the routine VSDpPrep:

```
In VSDp.f90 we have the routine for preparing inputs:

subroutine  VSDpprep  (IB,IE,iyrb,iyre,pCO2fv,expAl,lgKAloxv,modExc,lgExcMat, &
&                     thick,EBc0,Dep0,Wea0,Upt0,ECa0,EMg0,EK0,eqKv,KHBc,KAlBc)
  integer,         intent(in)    :: IB, IE, iyrb, iyre, modExc
  real,            intent(in)    :: pCO2fv(IB:IE),expAl,lgKAloxv(IB:IE),lgExcMat(6,6)
  real,            intent(in)    :: thick, EBc0
  type(Ions),      intent(in)    :: Dep0, Wea0, Upt0
  real,            intent(inout) :: ECa0, EMg0, EK0
  type(T_eqK),     intent(out)   :: eqKv(IB:IE)
  real,            intent(out)   :: KHBc, KAlBc
!DEC$ATTRIBUTES DLLEXPORT :: VSDpprep
```

the interface to this routines becomes after extraction with *extrcall* to a C++ interface:

```
typedef void (__stdcall *tVSDpprep) (int *,int *,int *,int *,float *,float *,
  float *,int *,float *,float *,float *,Ions *,Ions *,Ions *,float *,float *,float *,
  T_eqK *,float *,float *);
```

This definition is stored in the C++ header file of the VSDP class definition. During run time, we make the dll function available in C++ by:

```
VSDpprep = (tVSDpprep) GetProcAddress (pVSDdll,"VSDPPREP");
if (VSDpprep == NULL) {
  throw Exception ("Cannot find routine VSDPPREP in vsdp.dll");
}
```

Where pVSDPdll is a pointer to the dll obtained earlier using code like:

```
HMODULE pVSDdll = LoadLibrary("vsdp.dll");
if (pVSDdll == NULL) {
    ShowMessage("Fatal error : Cannot find model dll");
    exit(1);
}
```

3.4 Model parameters

Most of the model parameters have to be specified in the input file, but a few parameters for the soil organic matter model are fixed in the source code, to avoid that users will change these parameters asthese parameters are part of the Roth-C model. The fixed parameters are decomposition rates *k* (y^{-1}) and C/N-ratios per compartment, given in Table 3.

Table 3

Decomposition rates and C/N-ratios per compartment fixed in source code (Coleman and Jenkinson, 2014)

Compartment	k (y^{-1})	C/N
DPM	10	Calculated from incoming plant material
RPM	0.3	100
BIO	0.66	8.5 (in the code it is set to 15, with question mark!)
HUM	0.02	Calculated from the total amount of N in the soil and the C/N ratios of the other C pools
IOM	No decomposition	10

DPM and RPM decompose and form CO_2, BIO and HUM. The relationship between CO_2 and BIO + HUM is determined by a standard equation (section 1.7 in Coleman and Jenkinson (2014)). The ratio

between BIO and HUM is 46/54 (section 1.3 in Coleman and Jenkinson (2014)). This is also fixed in the code (Table 4).

The remaining fixed values in the source code are the conversion values to convert percentages of ions to equivalents. Finally the gas constant and CO_2 pressure in air are fixed values in the source code (Table 4).

Table 4
Fixed model parameters in source code

Parameter	Value (unit)	Description
frBIOM	0.46 (-)	Fraction BIO from BIO+HUM
cvN	0.713 (-)	N % --> eq: 1000/(M(N) *100)
cvCa	0.5 (-)	N % --> eq: 1000/(M(N) *100)
cvMg	0.823 (-)	Mg% --> eq: 1000/(M(Mg)/2*100)
cvK	0.256 (-)	K % --> eq: 1000/(M(K) *100)
cvP	0.32 (-)	P % --> eq: 1000/(M(P) *100)
Rgas	8.314 J/(mol*K)	gas constant
pCO2air	0.0004 (atm)	CO^2 pressure in air (400 ppm)

3.5 Model input

All inputs are described in the user manual and in the user friendly interface. Many input parameters have a default value if no value is specified in the input file. This is often set equal to 0. This is the case for e.g. element fluxes that enter the system, such as deposition, weathering, litter fall and uptake of nutrients by the vegetation. Also the initial C-pool is defaulted to 0.

Some inputs have other default values. The parameters for the initial bases saturation (bsat_0, ECa_0, EMg_0 and EK_0) is set default to-1. With this value, the initial base saturation is calculated with the assumption that there is equilibrium between the inputs of ions and the composition of the exchange complex within the first year of the simulation period. The exponent in the Al-hydroxide equilibrium (expAl) is default on 3 (i.e. gibbsite equilibrium), because with the gibbsite equilibrium generally good Al-concentrations are calculated (De Vries *et al.*, 1989).

For the dissociation of organic acids into organic anions in the soil solution, the three parameters are defaulted to values according to Oliver *et al.* (1983). The soil temperature is defaulted on 8 ^{o}C, a plausible value for Western Europe. The nitrification and denitrification rates are default set on 4 on the basis of expert judgement. Default value for Nupeff (the efficiency of N uptake) is set to 0.92, which is also expert judgement based on the fact that the system will always loose some nitrogen, even in systems where N is limiting.

3.6 Model output

All model output is sent to the subroutine 'monitor', which is described in Annex 2.

All possible model outputs are given in the output tabsheet of the GUI (Figure 4).

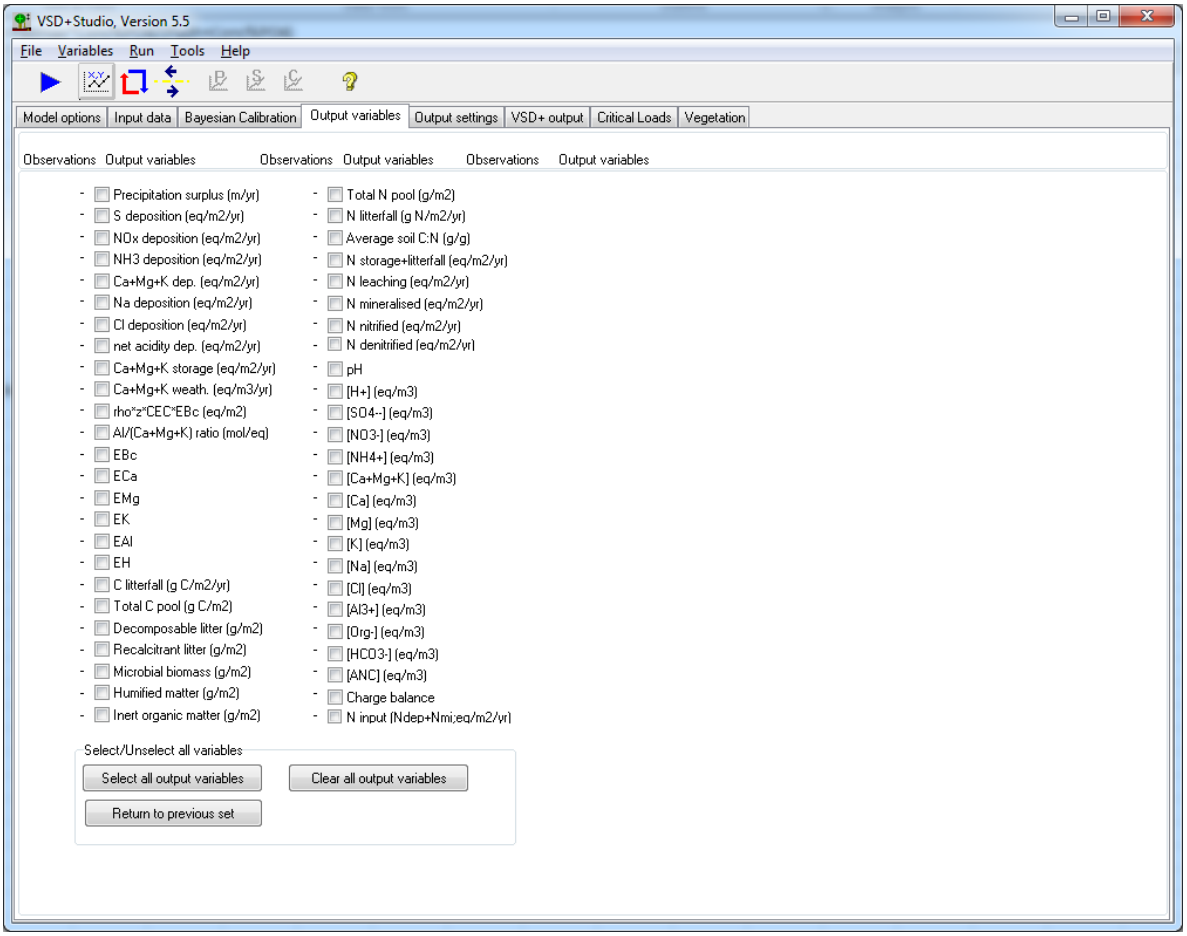

Figure 4 *Possible model output variables of VSD+*

The meaning of most variables is obvious. In Table 5 we give a description of the variables that may not so obvious or which are a combination of several output parameters.

Table 5
Description of output

Code	Output variable	Description or calculation
'ps'	Precipitation surplus (m/yr)	
'Temp'	Temperature (°C)	
'Sdep'	S deposition (eq/m^2/yr)	
'NOxdep'	NOx deposition (eq/m^2/yr)	
'NH3dep'	NH3 deposition (eq/m^2/yr)	
'Bcdep'	Ca+Mg+K dep. (eq/m^2/yr)	
'Nadep'	Na deposition (eq/m^2/yr)	
'Cldep'	Cl deposition (eq/m^2/yr)	
'Acidep'	net acidity dep. (eq/m^2/yr)	Sdep + NOxdep + Cldep – Cadep – Mgdep – Kdep – Nadep - NH3dep
'Bcupt'	net Ca+Mg+K uptake (eq/m^2/yr)	
'Bcwe'	Ca+Mg+K weathering (eq/m^3/yr)	
'Bcpool'	rho*z*CEC*EBc (eq/m^2)	
'AlBc'	Al/(Ca+Mg+K) ratio (mol/eq)	
'bsat'	Ebc	Exchangeable fraction of base cations (sum of Ca, Mg and K)
Eca'	ECa	Exchangeable fraction of Ca
'EMg'	EMg	Exchangeable fraction of Mg
'EK'	EK	Exchangeable fraction of K
'EAl'	EAl	Exchangeable fraction of Al

Code	Output variable	Description or calculation
'EH'	EH	Exchangeable fraction of H
'Clf'	C litterfall (g C/m^2/yr)	Amount of C input via litterfall
'Cpool'	Total C pool (g C/m^2)	Sum of C in all organic pools
'DPM'	Decomposable litter (g/m^2)	
'RPM'	Recalcitrant litter (g/m^2)	
'BIO'	Microbial biomass (g/m^2)	
'HUM'	Humified matter (g/m^2)	
'IOM'	Inert organic matter (g/m^2)	
'Npool'	Total N pool (g/m^2)	Sum of N in all organic pools, calculated by sum(Ctot(1:5)/CN(1:5))
'Nlf'	N litterfall (g N/m^2/yr)	Amount of N input via litterfall
'Cnrat'	Average soil C:N (g/g)	
'Nupt'	N storage+litterfall (eq/m^2/yr)	total N-uptake (=net N uptake + N litter fall)
'Nle'	N leaching (eq/m^2/yr)	Sum of NO_3 and NH_4 leaching, calculated by (cNO_3+cNH_4)*precipitation surplus
'Nmi'	N mineralised (eq/m^2/yr)	
'Nni'	N nitrified (eq/m^2/yr)	
'Nde'	N denitrified (eq/m^2/yr)	
'pH'	pH	
'cH'	[H+] (eq/m^3)	
'cSO4'	[SO4--] (eq/m^3)	
'cNO3'	[NO3-] (eq/m^3)	
'cNH4'	[NH4+] (eq/m^3)	
'cBc'	[Ca+Mg+K] (eq/m^3)	
'cCa'	[Ca] (eq/m^3)	
'cMg'	[Mg] (eq/m^3)	
'cK'	[K] (eq/m^3)	
'cNa'	[Na] (eq/m^3)	
cCl'	[Cl] (eq/m^3)	
'cAl'	[Al3+] (eq/m^3)	
'cOrg'	[Org-] (eq/m^3)	
cHCO3'	[HCO3-] (eq/m^3)	
'cAN	[ANC] (eq/m^3)	Concentration of Acid Neutralising Capacity
'balance'	Charge balance	Sum of all cations and anions in soil solution (eq.(1) in Posch and Reinds, 2009)

4 Users documentation

4.1 Scope and limitations

When VSD+ is downloaded and installed, a help file is included that can be viewed from the GUI, with a description of all model input and output. The user-interface is an easy-to-use shell that is described in section 3 of Posch and Reinds (2009).

The scope of the model is described in the introductions of Posch and Reinds (2009) and Bonten *et al.* (2016). The VSD model is designed to simulate the acidification (and recovery) of non-calcareous (unmanaged) soils and VSD+ is developed to simulate or predict effects of nitrogen deposition on carbon sequestration and on biodiversity through the use of an auxiliary model that simulates biodiversity metrics using VSD+ output, such as C/N ratios in the soil and NO_3 and NH_4 concentrations in the soil solution.

The papers about VSD and VSD+ also include descriptions of applications of both models. Other applications can be found in part 3 of the CCE status reports by 2011 and 2012 (CCE, 2011 and CCE, 2012), in which the National Focal Centres (NFCs) report their results. Several countries (e.g. Netherlands, Slovenia and Switzerland) have applied VSD+ to calculate both soil chemistry and critical deposition levels.

VSD+ is not tested on grassland and heathlands, but it should in principle be applicable for these systems as well, as long as they are dry. For wet systems like peatlands, the VSD+ model would have to be extended with anoxic soil-biochemical processes like iron and sulphate reduction, because these processes affect the pH. Also C and N turnover are not reduced for very wet conditions. This means that the current VSD+ model is not suitable to model very wet ecosystems (section 4 of Bonten *et al.* (2016)). Despite this restrictions for wet ecosystems, we have applied VSD+ to a wet heathland and a wet grassland to compare VSD+ with SMART2 (section 6.2.1) for two valuable vegetation types in the Netherlands. Results show that the model predictions were plausible. Probably as long as the groundwater level does not arise above soil surface, VSD+ can be used.

The VSD+ version that can be used for simulations on a single site can be downloaded (see meta-information).

4.2 Model applications

In most cases, VSD+ is applied on forest systems. In the paper about VSD+ (Bonten *et al*., 2016), three model applications on forest used for the model validation, can be found. Other model applications, can be found in 'Part 3' of CCE (2012) with applications by the NFC's of Austria (forest), Germany (forest and other vegetations), Slovenia (forest) and Switzerland (forest). In section 6.2 of this report applications on wet grassland and wet heathland are reported. An overview is given in Table 6.

Table 6
Examples of model applications

Site/region	Vegetation	Goal	Reference
Gårdsjön (Sweden)	Norway spruce, Scots pine	Model validation, N addition experiment, soil solution concentrations, C and N pools	Bonten *et al.,* 2016
Solling (Germany)	Norway spruce	Model validation, soil solution concentrations, C and N pools	Bonten *et al.,* 2016
8 plots in Austria	Different forest types (mainly Norway spruce and European beech	Test vegetation response to deposition	CCE, 2014
8 plots in Austria	Different forest types (mainly Norway spruce and European beech	Test vegetation response to deposition	CCE, 2014
32 sites in Switzerland	Forest	Test vegetation response to deposition	CCE, 2014
Different habitat types Netherlands	Forest, heathland and grassland	Habitat response to deposition	CCE, 2014
1 site, Netherlands	Wet heathland	Comparison with SMART2	Par 6.2.1 and CCE, 2012
1 site, Netherlands	Wet grassland	Comparison with SMART2	Par 6.2.1 and CCE, 2012
Netherlands	All Nature types	Calculation critical loads, which have to be delivered by PBL to CCE	CCE, 2015

4.3 Summary of calibrations, validations, testing and sensitivity analyses

VSD+ is applied by many different research groups in Europe. Most of the applications concern forests, but a few applications on grassland and heathland are described by researchers in the Netherlands. Calibrating the model is done by the automatic procedure, which is available in the GUI. Measured pH, C/N ratio and C pool can be used to calibrate exchange constants, weathering rates and initial C/N ratio and initial C pool.

Validations show that VSD+ is able to properly simulate the pH, base cation concentrations, nitrate concentrations, ammonium concentrations and organic C and N pools, especially in forest ecosystems.

The processes, described in the paper about VSD+, have been tested, by comparing model results with calculations in Excel. A few failures were found in the description in the paper (eq. 15, calculation of IOM and eq. 18 about the calculation of the initial pool of BIO). The way the processes were coded in the source code however, was correct.

Calculations of critical load for nitrogen with N availability as boundary condition were also successfully checked in Excel

A sensitivity analyses showed that the constant for the equilibrium between H^+ and Al^{3+} (lgKAlox) and the weathering rate of Ca (Cawe) are the parameters that determine the simulated pH. For base saturation, most important are the exchange constant between H^+ and Bc (lgKHBc) and the weathering rate of Ca. For C/N ratio litterfall of C and N and the uptake of N (Ngupt) are important influencing factors. The nitrate concentration strongly depends on the leaching flux (percol) and the net N input (input by NOxdep and NH3dep and removal by NGupt).

5 Testing

A limited number of tests have been performed to establish if VSD+ models the processes as described in its documentation. Code checking of the organic model part (CNRothC.f90) was done in October 2016. One issue was reported in Annex 4. A simple test of the calculation of critical loads is given in section 5.4.

5.1 Tests performed

The following tests have been performed, the eq. number(s) given for each test are those in the VSD+ documentation by Bonten *et al*. (2016), the VSD+ input file (see below) for each test is also given:

1. Computed pH from the charge balance (eq. 1), both for the Gapon and Gaines Thomas exchange models (vsdp_1.in (for Gapon), vsdp_gt_1.in (for Gaines Thomas)).
2. Concentration of an ion that is a tracer (eq. 2); used [SO_4^{2-}] to test, using a sudden decrease in sulphur input halfway the simulation period (vsdp_2.in).
3. H^+ and AL^{3+} sorbed at the exchange complex (eq. 2) for Gaines Thomas and Gapon exchange models (vsdp_6.in (Gaines Thomas), vsdp_7.in (Gapon)).
4. Computation of the carbon pool (eq. 4,5,8,16,17,19) (vsdp_3.in).
5. Carbon in the IOM pool (eq. 15) (vsdp_3.in).
6. N mineralisation (eq. 11) and C/N ratio in the DPM pool (eq. 12) (vsdp_4.in); for this test additional, detailed, results were required from the model that are not in the available output. These were obtained by debugging the model.
7. N nitrification (eq. 21) and denitrification (eq. 22) (vsdp_5.in).

For each test, an input file for VSD+ has been made that specifies the inputs needed for the specific test. In this input file, there is a reference to a so-called monitor file, named after the VSD+ input file with file extension *mon*, that specifies which model outputs are written to the output file (in ascii format). Output files are also named after the input files, but with file extension *out* (vsdp_1.in in combination with vsdp_1.mon produces vsdp_1.out). These output files have been loaded into excel data sheets, in which the tests have been performed: in excel, we computed the output variable of interest independently, and compared these results with the model outputs produced by VSD+. Results were compared for each year within a simulation period between 1960 and 2010.

In Annex 3, the results of each of the tests are provided. The left part of each sheet consists of the VSD+ output file that was loaded, including the header that specifies which output parameters were written to the file, with their units of measure. The column indicated with the green colour, is the column that provides the VSD+ output parameter from the output file that was tested for correctness. The column with the blue colour is the value of this output parameter that was independently computed in Excel, from other output parameters from the model. Cells with the colour light brown are cells that hold information on model parameters obtained from the VSD+ input file that are sometimes needed to perform the test. Occasionally, these cells are also used to convert such parameters to the proper units, as is done within VSD+. If the test succeeds, the values in the green and blue columns should be identical: the ratio was computed for each test and is displayed in orange (values should be 1.00).

The modelling of the C/N ratio in some of the organic matter pools has not been tested, because it is modelled in VSD+ using iterative procedures (modified 4th-order Runga-Kutta procedure based on Numerical Recipes (2007)).

5.2 Results

Results of the tests 1-7 confirm that VSD+ computes results according to its specifications as described in Bonten *et al.* (2016), except for test number 5. This test revealed an error in the

documentation; after consulting the source of this equation (Falloon *et al.*, 1998), and re-deriving it for VSD+, eq. 15 should read

$$\mathrm{IOM} = 0.049 \cdot \mathrm{SOC}_{\mathrm{ini}}^{1.139} \cdot 100^{-0.139} \qquad (15)$$

In the paper the constant was specified to be 0.026, which is wrong. The equation was however correctly implemented in the VSD+ source code:

```
Cpool(5)=  (0.049 * (Ctot/100)**1.139)*100
```

Which is equivalent to the correct eq. 15.

Test 7 showed that the denitrification flux in the first simulation year is about 12% different from its independently computed value. This difference disappears in the second simulation year. It is likely to be due to the fact that in the test we assumed all uptake is in the form of NH_4, which may not be the case during initialisation of the model, but to confirm this would require a more detailed analysis.

5.3 Storage of testruns

The testruns are stored on the SMART-share: \\WUR\dfs-root\ESG\shares\SMART and located in the subdirectory: VSDp\modelquality\testfiles. These tests are included in the repository of VSD+, together with the source codes of VSD+. The check on the model results is done in the excel file 'AllVSDpTestresults.xlsx'. This file has eight tabsheets with each one of the in section 5.1 described tests per tabsheet. All of these tests have their own input file (also given in section 5.1) and output. The output can easily be copied in the excelfile.

5.4 Test calculation of critical loads

The testing of the calculation of the critical loads has been done separately. When the critical N availability is set as the boundary condition, which is the base of the ciritcal load values in AERIUS, the PAS' calculation tool for calculating the amount of room available for nitrogen deposition from new or expansion of current activities, the critical load is calculated with equation (SS15) in the description of the steady state calculation in the Help-file:

$$CL(N) = N_{av,crit} - N_{lf} - N_{fix} - N_{seep}$$

Where $N_{av,crit}$ is the critical N availability, N_{lf} is is N input via litter fall, N_{fix} is N fixation and N_{seep} is N input via upward seepage (all in the same units e.g. eq.m^{-2} or kmol.ha^{-1}. This equation is tested in excel, for all plots with nature in the Netherlands. Except for small differences due to rounding off, the results were equal (Table 7).

Table 7
Few results of the testing critical load for N availability

Navcrit	CLmaxS	CLminN	CLmaxN	CLnutN	nANCcr	lgKAlBc	lgKHBc	Nlf	Nseep	Nim	Nup	CLN_ca	check
1.036	23.6	678.8	705	3429.6	0	0.668	4.189	0.693	0	0	0.761	3430	1.00
1.072	23.6	678.8	705	3533	0	0.668	4.189	0.719	0	0	0.787	3530	1.00
1.072	289.3	509.1	897.1	3533	0	-2.189	6.397	0.719	0	0	0.77	3530	1.00
1.072	23.6	678.8	705	3533	0	0.668	4.189	0.719	0	0	0.787	3530	1.00
1.036	23.6	678.8	705	3429.6	0	0.668	4.189	0.693	0	0	0.761	3430	1.00
1.072	23.6	678.8	705	3533	0	0.668	4.189	0.719	0	0	0.787	3530	1.00
1.036	23.6	678.8	705	3429.6	0	0.668	4.189	0.693	0	0	0.761	3430	1.00
1.072	23.6	678.8	705	3533	0	0.668	4.189	0.719	0	0	0.787	3530	1.00
1.036	23.6	678.8	705	3429.6	0	0.668	4.189	0.693	0	0	0.761	3430	1.00

6 Calibration and validation

6.1 Calibration

Reinds *et al.* (2008) describe the calibration procedure which is used for VSD+. Parameters that can be calibrated with the automatic procedure are: the exchange constants KHBC and KAlBC, the initial C-pool, the initial C/N-ratio and weathering rates of Calcium (Ca), Magnesium (Mg) and potassium (K). This calibration procedure can be used if enough measurements (pH, base saturation and/or concentrations of Ca, Mg and/or K for the calibration of the Exchange constants and the weathering rates; measurements of the C-pool and C/N-ratio are required to calibrate initial C-pool and initial C/N-ratio) are available for calibration. Bonten *et al.* (2016), calibrated only the exchange constants using measurements of pH, base saturation and concentrations of the base cations Ca, Mg and K. Other model calibrations, can be found in 'Part 3' of CCE (2012) with applications by the NFC's of Austria, Germany, Slovenia and Switzerland.

When VSD+ is used to calculate critical loads (CLs) the above-described calibration is also used for a single site calculation and when pH, Cpool and C/N are measured. When these measurements are not available, VSD+ is not calibrated.

6.2 Validations

We have validated VSD+ on sites with measured soil moisture concentrations and organic pools of carbon (C) and nitrogen (N) (section 6.2.1) and compared critical load (CL) calculations with former CL calculations with SMART2 and empirical critical loads (section 6.2.2).

The validation on sites with measured soil moisture concentrations and C and N pools showed that VSD+ was able to reproduce the observed trends over more than 30 years and levels of pH, base cations and NO_3 and NH_4 concentrations satisfactorily. Even on wetter ecosystems, VSD+ was able to calculate plausible C and N pools, pH and concentrations of NO_3.

Calculated CLs with VSD+ match with former calculations with SMART2 and with the empirical values of the main habitat types in the Netherlands.

6.2.1 Soil moisture concentrations and C/N-ratio

Bonten *et al.* (2016) describe a validation of VSD+ on three different forest sites. Both the absolute values as well as trends over time of the $NO_3$and NH_4 concentrations and C/N ratios were well simulated by VSD+. Acidification and recovery from acidification by VSD+ were well modelled as the model was able to simulate both the decrease and increase in pH over time.

In part 3 of CCE (2012) a comparison is made between SMART2 and VSD+ applications for three vegetation types: forest on a dry sandy soil, grass on a wet sandy soil and heath on a wet peaty soils (Figures 5-7). Since in VSD+ the initial C-pool is calibrated using measured C-pool and C/N ratio, the simulated values of C-pool and C/N-ratio by VSD+ match better the measured values than those of SMART2 as SMART2 was not calibrated. Exchange constants for VSD+ are also calibrated and therefore pH is also better simulated than with SMART2. Although not developed for wet systems, results show that the model predictions were plausible. Probably as long as the groundwater level does not arise above soil surface, VSD+ can be used.

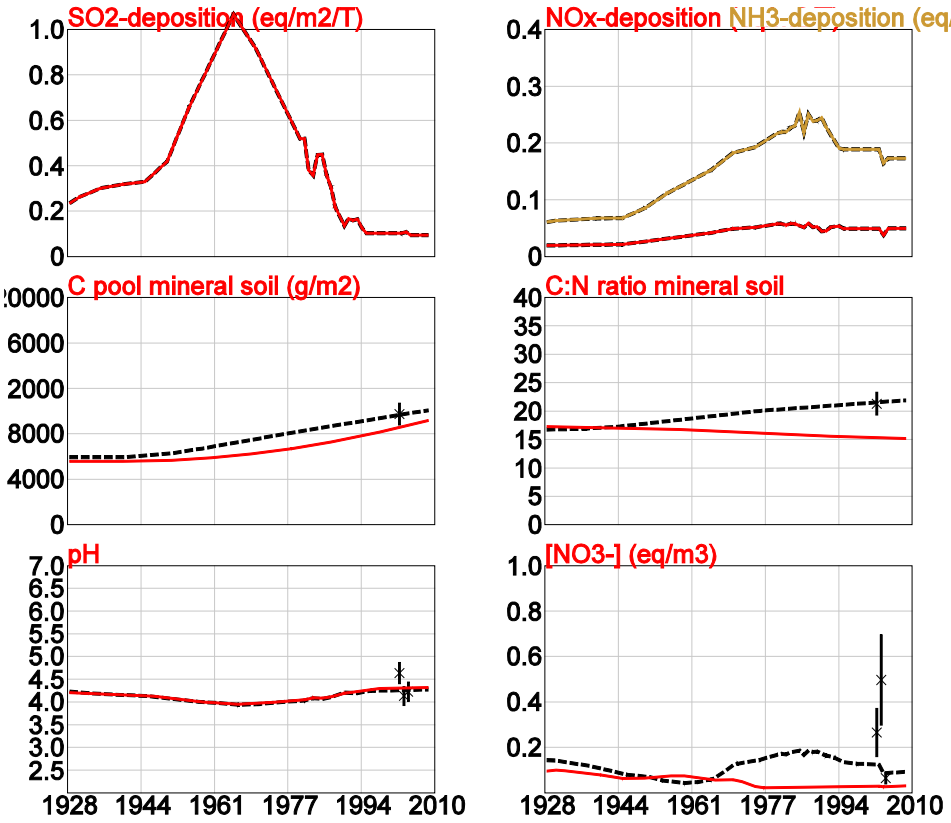

Figure 5 *C-pool, C/N-ratio, pH and [NO_3] calculated by SMART2 (___) and VSD+ (---) on dry sand, Zeist*

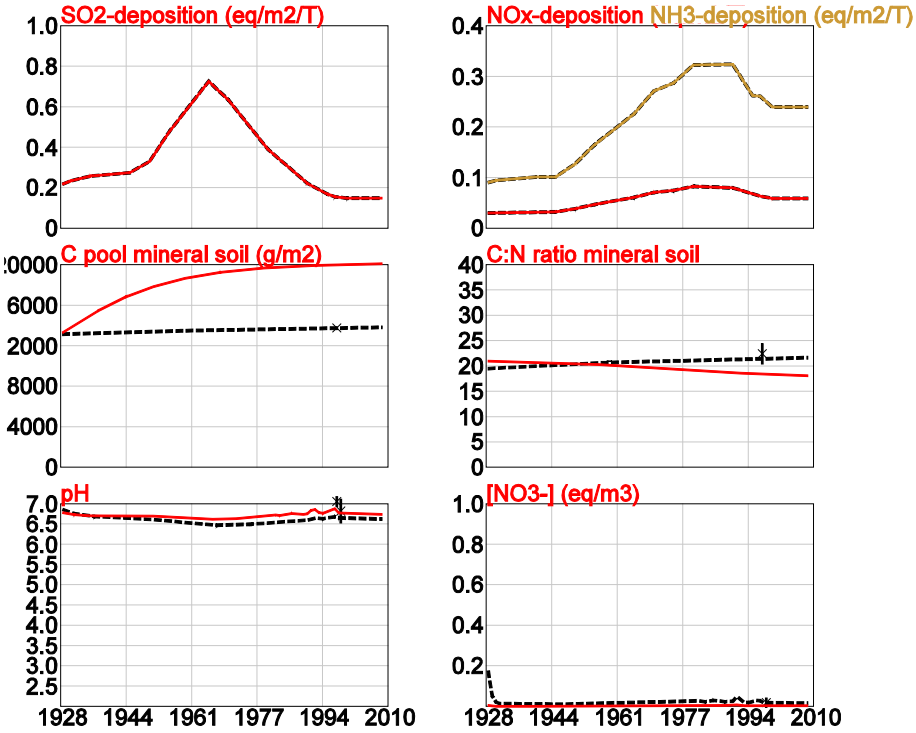

Figure 6 *C-pool, C/N-ratio, pH en [NO_3] calculated by SMART2 (___) and VSD+ (---) on wet grassland, Lemselermaten*

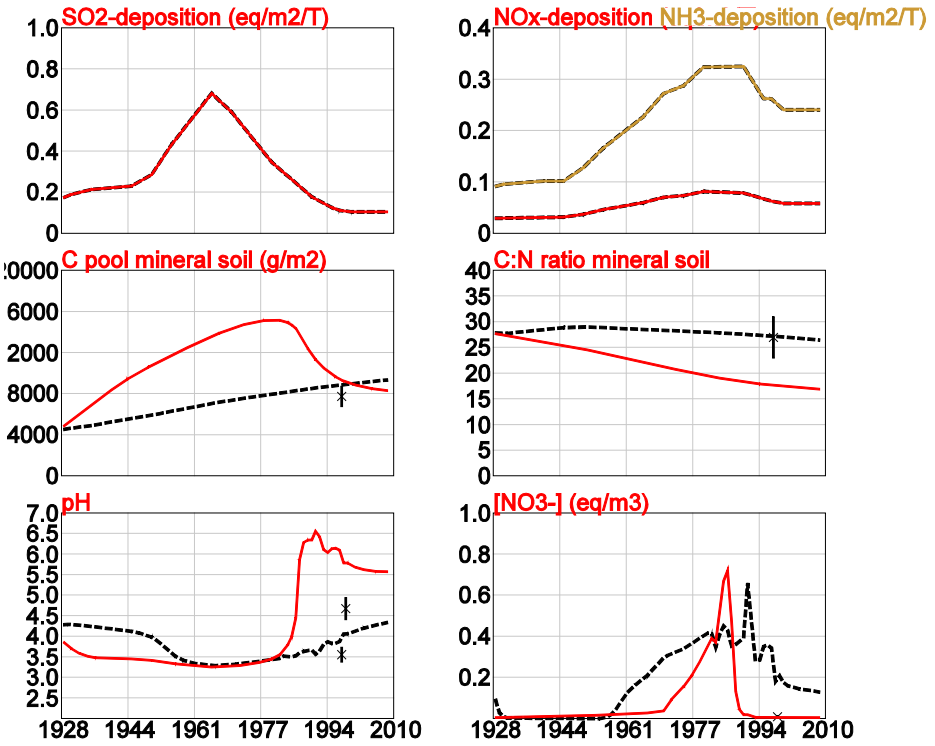

Figure 7 *C-pool, C/N-ratio, pH and [NO_3] calculated by SMART2 (___) and VSD+ (---) on wet heath, Korenburgerveen*

6.2.2 Critical loads

In addition to the calculation of soil moisture concentrations, also calculations of critical loads of SMART2 were compared with those of VSD+. The critical loads calculated with SMART2 by Van Dobben *et al*. (2006), were reproduced with VSD+, for most of the vegetation associations, when the same boundary conditions (minimum pH and maximum N availability by association) were used and when all inputs were as similar as possible. It was not always possible to achieve the required pH and N availability, because in some ecosystems this would require a negative deposition. In those cases, the required pH and/or N availability were set to the closest possible pH and N availability, so the pH and N availability with zero N deposition. These closest values were used in the VSD+ calculations for the comparison with SMART2. This is shown in Figure 8 in which a comparison is made between the calculated critical loads for nitrogen (CLN) by SMART2 and VSD+.

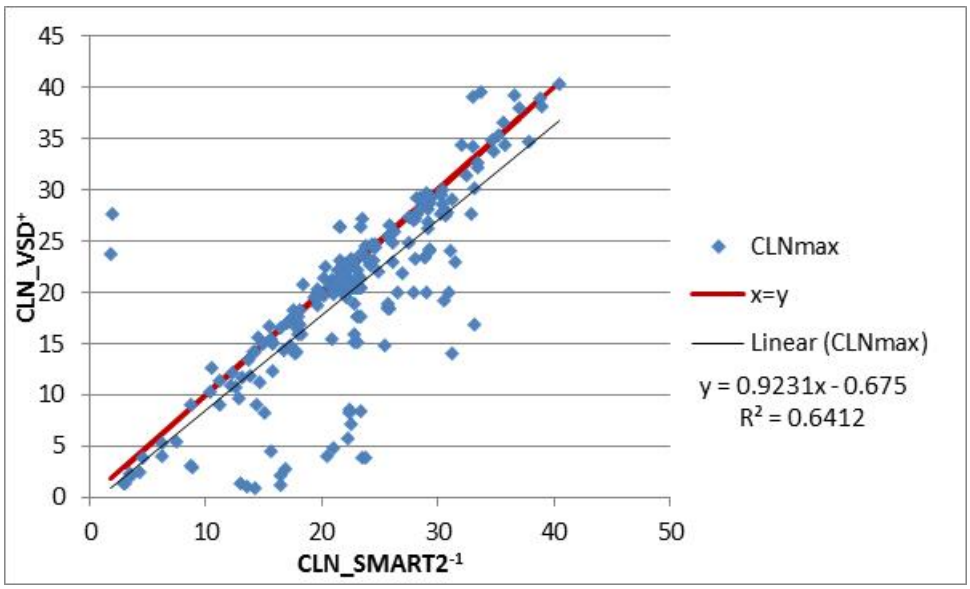

Figure 8 *CLN calculated with VSD+ based on best possible pH and N-availability calculated by SMART2 (instead of required) against SLN calculated with SMART2^{-1}.*

We also made a comparison of VSD+ critical loads and empirical ranges (CCE, 2015). For those habitat types where a comparison could be made, the calculated CL are within the empirical range, see Table 8.

Table 8

Critical loads in database CCE (calculated by VSD+) compared with empirical ranges and critical loads used in Dutch policy (PAN)

Type	Habitat type	Critical load (N, kg ha^{-1} yr^{-1})		
		Database CCE	***Empirical range***	***PAN***
Bogs	H7110	6	5-10	7
Dune grasslands	H2130	9	8-15	10
Dry heathland	H4030	15	10-20	15
Salt marches	H1330	29	20-30	22
Dry nutrient-poor forest	habitat for protected animals	16	10-20	15

6.3 What is not validated?

Most validations concern the calculation of soil moisture concentrations and C/N ratios of the soil. Nitrogen fluxes such as nitrogen mineralization, nitrification and denitrification are not yet validated separately. It is important to model these fluxes well, because they determine the nitrogen availability for the vegetation. Also other element fluxes, such as mineralization of base cations are not validated, but these are more affected by the model input (via deposition and litter production) than by internal processes.

6.4 Shortcomings

Bonten *et al.* (2016; end of section 4) describe a number of shortcomings. It is mentioned that the model is not extensively tested is on wet systems and that some anaerobic processes need to be included for very wet systems, especially for peatlands. They also mention that there is no feedback between soil and vegetation. Higher availability of nutrients in the soil should lead to higher nutrient contents in vegetation, but that feedback is not included in VSD+. By coupling VSD+ to e.g the SUMO model (Wamelink *et al.*, 2009) it is however possible to include the feedback between soil and vegetation.

7 Sensitivity analyses

A simple sensitivity analysis was carried for VSD+. This analysis shows how sensitive model results are for changes in model input parameters. In this analysis we analysed the sensitivity of the simulated pH (pH), base saturation (bsat), CN ratio (cnrat), and nitrate concentration (cNO3), the first two outputs being indicative for acidification and the latter two for eutrophication of soils. Also the sensitivity of the critical loads for sulphur (CLmaxS) and of nitrogen (CLmaxNO, CLmaxNH) were determined. For CLmaxS we use a critical pH value as a criterion, for critical loads for N we used a critical nitrate concentration as well as a critical N availability. The analysis was carried out using the SimLab software package (version 2.2.1, https://ec.europa.eu/jrc/en/samo/simlab) that uses a Monte-Carlo procedure to establish the sensitivity of model outcome to model input.

7.1 Methods

7.1.1 Parameter distributions and uncertainties

For each of the VSD+ input parameters a distribution type and distribution was defined, were the average values are based on those at the Hubbard Brook site in the North-east of the United States of America (Todd McDonnell, pers. comm.), see Table 9.

Table 9

VSD+ parameters and their assumed uncertainty

Parameter	Type	Average/ minimum	Std.dev./ maximum
thick	Normal	0.5	0.1
bulkdens	Normal	1.3	0.1
Theta	Normal	0.35	0.05
pCO2fac	Normal	30	5
CEC	Normal	30.4	10
lgKAlBc	Normal	0.3	0.3
lgKHBC	Normal	-3.15	0.311
lgKAlox	Normal	8	1
cRCOO	Normal	0.02	0.01
TempC	Normal	5	0.2
percol	Normal	0.3	0.05
Cawe	Normal	0.04	0.0158
SO2dep	Normal	0.05	0.005
NOxdep	Normal	0.05	0.005
NH3dep	Normal	0.02	0.005
NGupt	Normal	0.7	0.15
Caupt	Normal	0.005	0.001
Clf	Normal	540	100
Nlf	Normal	10	2
rfmin	Uniform	0.8	1
rfnit	Uniform	0.8	1
rfmiR	Uniform	0.8	1
Clayct	Uniform	2	8

Not for all input parameters the uncertainty was defined: for example the effects of weathering of individual cations on output was aggregated into Ca weathering, as Mg and K in VSD+ are included in the same processes as Ca is (weathering, uptake, exchange, leaching) and are likely to show the same sensitivity. For most parameters the uncertainty was set by expert judgement. Uncertainty in exchange constants was obtained from De Vries and Posch{De Vries, 2003 #1839}. Uncertainty in the reduction factors (rfmin, rfnit, rfmiR) was based on insights obtained from computed values with the MetHyd model: in well drained soils values for these factors will be mostly between 0.8 and 1.0.

Some parameters were assumed to be correlated: SO_x and NO_x deposition (correlation coefficient (cc) = 0.7) were the correlation was based on the correlation between these parameters in European data sets, Clf and Nlf (cc = 0.8) as the C/N ratio in litterfall is within clear limits, NGupt and Caupt (cc=0.8) because trees take up nutrients in ratios with little variance. These correlations have been used in the sampling procedure.

7.1.2 Sampling

From the set of uncertain input parameters, a sample of 3000 realisations was obtained using Latin Hybercube sampling. This stratified sampling method is superior to random sampling as it is able to achieve a better coverage of the sample space of the input factors with a limited sample size. To verify correct sampling, one can examine the distribution of the parameters in the realised sample:

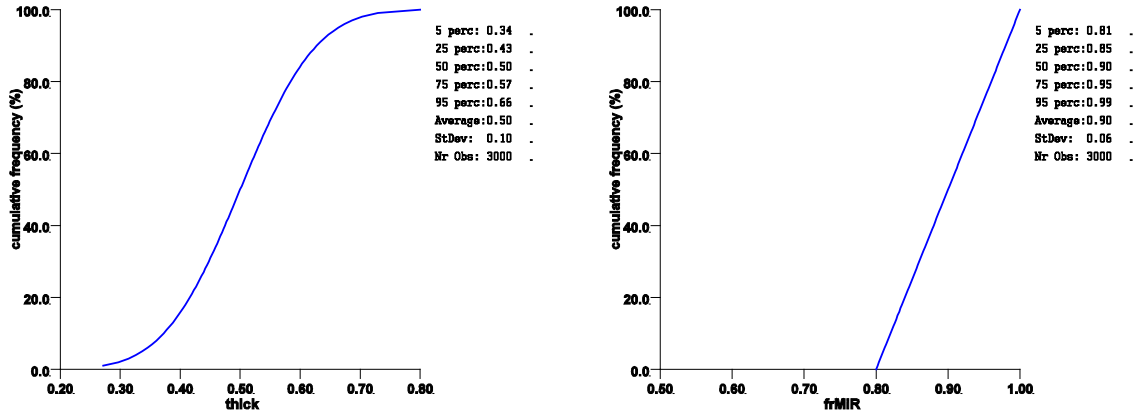

Figure 9 *Cumulative distributions obtained from the realised sample (sample size 3000).*

Comparing Table 9 and Figure 9 shows that the sampling reproduces the predefined distributions perfectly.

7.1.3 Running the model

Using the standard VSD+ dll's, a command line executable version of VSD+ was developed that runs VSD+ consecutively for each of the 3000 lines in the sample file: parameter values are read from these lines and used as input for the VSD+ model. Simulations were performed for the period between 1880 and 2050. Simulated values for pH, base saturation CN ratio and nitrate concentration as well as computed critical loads for S and N based on each of the 3000 samples were written to an output file according to the format prescribed by the SimLab software.

7.2 Results of the analysis

The purpose of sensitivity analysis is to determine the relationships between the uncertainty in the inputs and that in the resultant dependent variables. With the Monte Carlo procedure, propagation of the sample through the model creates a mapping from analysis inputs to analysis results. Once this mapping is generated and stored, it can be explored in many ways to determine the sensitivity of

model predictions to individual input variables. SimLab performs seven different statistical tests to establish the relationship between model input and model output. Here we have used the Spearman coefficient of correlation, as this is a suitable measure for non-linear models. SimLab computes the coefficients based on the sample and the model output and also ranks them. Spearman correlation coefficients were computed for the four model outcomes and for the simulation years 2000 and 2050 (Table 10) and for the critical loads for sulphur (S), nitrogen oxide (NO) and ammonia (NH) with two different boundary conditions (Table 11).

Table 10

Ranks based on Spearman correlation coefficients of the VSD+ parameters for the four model outcomes for the years 2000 and 2050.An asterisk indicates a non-significant correlation (90% confidence interval). The green shaded cells show the five most sensitive variables.

Variable	pH		Bsat		CNrat		cNO3	
	2000	2050	2000	2050	2000	2050	2000	2050
thick	11	7	9	5	14*	13*	7*	8*
bulkdens	13*	14*	13*	16*	7*	7*	22*	17*
Theta	17	16	17	14	21*	21*	8*	9*
pCO2fac	14*	13*	14*	13*	15*	15*	13	14
CEC	7*	12*	4*	11*	10	10	14*	13*
lgKAlBc	5	10	1*	1*	12*	11*	18*	15*
lgKHBC	22*	21*	18*	17	23*	23*	20*	21*
lgKAlox	1	1	3*	3*	19*	19*	15*	18*
cRCOO	21*	22*	16*	15*	18*	18*	16*	16*
TempC	23*	23*	19*	20*	17*	17*	21*	20*
percol	12	11	15*	22*	20*	20*	1*	3*
Cawe	2	2	2	2	22*	22*	19*	22*
SO2dep	4*	6*	6*	8*	8*	8*	10	10
NOxdep	9*	9*	10*	10*	9*	9*	5	6
NH3dep	15*	15*	12*	12*	6*	6*	4	5
rfmin	18	18*	22*	23*	13*	14*	17*	19*
rfnit	20*	19*	21*	18*	11*	12*	11*	11*
rfmiR	16*	17*	23*	19*	5*	5*	12	12
NGupt	3	3	5	4	1	1	2*	1*
Caupt	8	5	7	6	2	2	3*	2*
Clf	10*	8*	11*	9*	4*	4*	9	7
Nlf	6*	4*	8*	7*	3*	3*	6	4
Clayct	19*	20*	20*	21*	16*	16*	23*	23*

For pH, the constant for the equilibrium between H^+ and Al^{3+} in the soil solution (lgKAlox) and the weathering rate of Ca (Cawe) are the most important parameters. Ca weathering buffers acidic input and thus directly influences pH. Also relevant (especially in 2000) is the acid input (SO2dep) and the removal of N (NGupt) as this uptake also takes away the incoming acidity through nitrogen. For base saturation, most important are the exchange constant between H+ and Bc (lgKHBc) and the weathering rate of Ca. Also important is lgKAlox as this influences the concentration of H^+ in the soil solution and thus the equilibrium of H^+ and BC at the exchange complex. For CN ratio litterfall of C and N and the uptake of N (Ngupt) are important influencing factors. Ca uptake (Caupt) is ranked high in the Spearman test, but scores very low in the rank correlations tests. The high rank in this Spearman scores is an artefact caused by the assumed strong correlation with the N uptake, as there is also no conceptual way Ca uptake should influence the C/N ratio. This was confirmed by a run where the correlation was set to zero: then Caupt has no correlation with C/N ratio and has the lowest

rank (23) of all parameters in the Spearman test The nitrate concentration strongly depends on the leaching flux (percol) and the net N input (input by NOxdep and NH3dep and removal by NGupt). Again, the high rank of Caupt is caused by the correlation with NGupt, but has no real meaning. In general, there is a strong similarity between the two simulation years with respect to the most relevant input parameters.

Table 11

Ranks based on Spearman correlation coefficients of the VSD+ critical loads. An asterisk indicates a non-significant correlation (90% confidence interval). The green shaded cells show the five most sensitive variables.

Variable	CLmaxS	CLmaxNO(NO_3)	CLmaxNO(Nav)	CLmaxNH(NO_3)	CLmaxNH(Nav)
thick	17*	8*	14*	9*	13*
bulkdens	15*	16*	11*	12*	10*
Theta	20*	23*	16*	22*	16*
pCO2fac	21*	9*	17*	13*	19*
CEC	8*	14*	10*	8*	12*
lgKAlBc	3	7*	6	4	8
lgKHBC	22*	10*	15*	11*	17*
lgKAlox	1	1	1	1	1
cRCOO	13*	5	7	7	7
TempC	16*	19*	20*	10*	21*
percol	2	4	3	2	3
Cawe	12*	18*	13*	16*	14*
SO2dep	10*	13*	12*	15*	11*
NOxdep	14*	12*	18*	20*	18*
NH3dep	4	15*	21*	19*	20*
rfmin	6*	2	4	3	5
rfnit	7*	3*	9*	5*	6*
rfmiR	9*	22*	22*	21*	23*
NGupt	23*	20*	19*	18*	22*
Caupt	19*	11*	23*	14*	15*
Clf	5*	17*	5	17*	4
Nlf	11*	21*	2	23*	2
Clayct	18*	6	8	6	9

For the maximum critical of S based on the pH criterion, the constant for the H-Al equilibrium in the soil (lgKAlox) is the dominant parameter; this is obvious as at given acidity input this parameter determines the amounts of Al^{3+} and H^+ in the soil solution and thus the pH. The other important parameter is the leaching flux (percol) that determines the amount of acidity leaching. For the critical loads for N based on a critical nitrate concentration, lgKAlox is also dominant as it influences the steady state pH and with that the reduction functions for nitrification and denitrification which are important processes for ClmaxNO and CLmaxNH. If the critical load of N is based on the N availability, the litterfall flux of N becomes an important parameter as this determines most of the N available in the soil. For critical loads of N, the leaching flux is always an influential parameter, because it influences the N leaching from the soil and thus directly the critical load.

In Annex 5, extra information is given about uncertainties of the critical loads, which are not caused by uncertainties in the VSD+ calculations, but due to uncertainties of the boundary conditions.

7.3 Conclusions

The Al equilibrium constant (lgKAlox) and the weathering rate of Ca are the most sensitive input parameters for the calculation of pH and base saturation. These outputs are also sensitive to N uptake. N uptake is the most sensitive input parameter for CN ratio and next to percolation also for the NO_3 concentration.

So, an accurate estimate of uptake of N and Ca is thus required for an adequate simulation of N related output and, to a lesser extent, also for acidity related output (pH and base saturation). For soil acidity (pH, base saturation), an accurate estimate of Ca weathering and lgKAlox is required. Also a the exchange constant between H+ and Bc (lgKAlBc) is important.

The critical loads are most sensitive to lgKAlox, the leaching flux (percol) and reduction factor for mineralisation (rfmin). A accurate estimate of the litter fall flux (both C and N) is also important for plausible critical loads.

Litterfall and uptake are quite important for adequate simulations of soil moisture quality, organic C and N pools and critical loads calculations, which was the reason to make a tool (GrowUp) to provide this input. This tool is also available on the website http://wge-cce.org/Methods_Models/Available_Models.

Gathering data for model parameterisation should be focussed on Al equilibrium, cation exchange, weathering, mineralisation and water leaching fluxes.

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Justification

This study was carried out and supervised by Janet Mol and Gert Jan Reinds (Wageningen Environmental Research. The research methods and research approach has been supervised by the auditors Janien van der Greft, Geerten Hengeveld and George van Voorn of the Statutory Research Tasks Unit for Nature & the Environment. Their comments have been considered and incorporated as much as possible in this final report.

Annex 1 Interfaces of the subroutines

VSDpin

```
! Calls READINP, performs IA inputs, does some conversions and displays/writes
! messages (mostly for default settings).
!
! INPUT:
! datfil ..... name of input data file for VSD (if blank asked interactively)
! msg ........ I/O unit for messages;
!              if msg<=0 no messages, if msg=6: written to screen
! msgfil ..... name of file for messages (not used for msg<=0 or msg=6)
! IB ......... first index of time series vectors
! IE ......... last index of time series vectors
!
! OUTPUT:
! Infobyte ... byte-vector holding user-specified site info
! iyrb ....... first year of simulation (iyrb >= IB)
! iyre ....... last year of simulation (iyre <= IE)
! eqKv() ..... chemical (equilibrium) 'constants'
! thick ...... soil thickness (m)
! rho ........ bulk density (g/cm3)
! thetav() ... volumetric water content of the soil (m3/m3)
! CEC ........ cation exchange capacity of the soil (meq/kg)
! ECa0 ....... initial exchangeable fraction of Ca (if EMg0<0 or EK0<0 then initial base saturation)
! EMg0 ....... initial exchangeable fraction of Mg
! EK0 ........ initial exchangeable fraction of K
! parentCa ... if >=0 simulate calcareous soil; value of parentCa (<=1) is fraction of Ca
!              in limestone (rest is Mg, as e.g. in dolomite); if <0: non-calcareous soil
! ctclay ..... clay contents of the soil (%)
! modExc ..... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
! KAlBc ...... selectivity constant for Al-Bc exchange
! KHBc ....... selectivity constant for H-Bc exchange
! Cpool0 ..... initial amount of C in topsoil (g/m2)
! CNrat0 ..... initial C:N ratio in topsoil (g/g)
! pKpar() .... 1-3 parameters of (Oliver-type) mono-protic organics model:
!              pK = par(21)+par(22)*pH-par(23)*pH^2
! coacid() ... total concentration of organic acids (m*DOC) (mol/m3)
! temp() ..... mean annual soil temperature (oC)
! ps() ....... precipitation surplus (runoff) (m/yr)
! Wea()%X .... weathering rate of X (X=Ca,Mg,K,Na) (eq/m3/yr)
! Upt()%X .... net uptake of X (X=Ca,Mg,K) (eq/m2/yr)
! Dep()%X .... deposition of ion X (eq/m2/yr);
!              X = SO4, NO3, NH4, Ca, Mg, K, Na, Cl
! Cpool0 ..... initial amount of C in topsoil (g/m2)
! Nlf ........ litterfall N (g N/m2/yr)
! QIlf() .... Quality index of litterfall (-)
! CN() ....... C:N ratio of C pools (g/g)
! kni ........ maximum nitrification rate at Tref (yr-1)
! kde ........ maximum denitrification rate at Tref (yr-1)
! Clf() ...... C litterfall (g C/m2/yr)
! rfmi()...... reduction function of moisture, drought and temperature for mineralisation (-)
! rfni()...... reduction function of moisture, drought and temperature for nitrification (-)
! rfde()...... reduction function of moisture, drought and temperature for denitrification (-)
! fN2Oni ..... N2O emissions as fraction of nitrification (-)
! fN2Ode ..... N2O emissions as fraction of denitrification (-)
! Nfix() ..... N fixation (eq/m2/yr)
! Nupeff ..... uptake efficiency of available N (-)
! Sadmax ..... maximum SO4 adsorption capacity (meq/kg)
! Sadh ....... half-saturation constant for SO4 sorption (eq/m3)
! Padmax ..... maximum PO4 adsorption capacity (meq/kg)
! Padh ....... half-saturation constant for PO4 sorption (eq/m3)
! - other output:
! iss ........ option for desired sea-salt SO4 (Correction not done in VSDin!):
!              =0: no sea-salt correction
!              =1: correct using Cl (i.e. Cl*=0)
!              =2: correct using Na (i.e. Na*=0)
! monfil ..... file for MONITOR
! OBSv() ..... observations
! errbyte .... byte-vector for error messages
!
```

Readinp

```
! Reads input data for VSD or SMART|2 from INP%file and, if not found, sets
! default values for some of them.
!
! INP
!  %model .... name of model ('VSD','SMART','SMART2')
!  %file ..... name of input data file
!  %path ..... path extracted from %file
!  %nvars .... number of keywords/variables incl. default ones
!  %key() .... keywords for variables
!  %line() ... lines with variables
!  %got() .... =.true., for those variables which were read from %file
!              or got default values
!  %def() .... =.true., if a default value has been set
!
! INPUT:
! nout ...... number of output/observation variables
! Varout() .. names, definitions & y-values of 'nout' variables;
!             not needed if nout<=0
! mdx ....... index function
! IB ........ first index of time series vectors
! IE ........ last index of time series vectors
!
! OUTPUT:
! Infobyte .. byte-vector holding user-specified site info
! iyrb ...... first year of simulation (integer)
! iyre ...... last year of simulation (integer)
! mstep ..... number of sub-periods within a year (integer)
! iss ....... option for seasalt correction:
!             =0: no seasalt correction
!             =1: correct using Cl (i.e. Cl*=0)
!             =2: correct using Na (i.e. Na*=0)
! thick ..... soil thickness (m)
! rho ....... bulk density (g/cm3)
! thetav() .. volumetric water content of the soil (m3/m3)
! pCO2fv() .. partial CO2-pressure in soil solution as multiple of pCO2(atm) in air
! CEC ....... cation exchange capacity of the soil (meq/kg)
! ECa0 ...... initial exchangeable fraction of Ca
! EMg0 ...... initial exchangeable fraction of Mg
! EK0 ....... initial exchangeable fraction of K (VSD only)
! EBc0 ...... initial exchangeable fraction of Ca+Mg+K (if ECa0, EMg0, EK0 not given)
! modExc .... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
! lgExcMat .. 6x6 matrix of log10 of CatExc selectivity constants:
!             lgExcMat(i,j) for lgKij, i,j=H,Al,Ca,Mg,K,Na (Bc=Ca);
!             e.g. lgExcMat(1,3) = lgKHBc
! expAl ..... exponent in [Al] = KAlox*[H]^expAl
! lgKAloxv() . log10 of Al equilibrium constant ((eq/m3)^(1-expAl))
! Sadmax .... maximum SO4 adsorption capacity (meq/kg)                !!!
! Sadh ...... half-saturation constant for SO4 sorption (eq/m3)
! Nim0v() ... C:N-independent N immobilization (eq/m2/T)
! Cpool0 .... initial amount of C in topsoil (g/m2)
! CNrat0 .... initial C:N ratio in topsoil (g/g)
! CNmin ..... minimum C:N ratio in topsoil (g/g)
! CNmax ..... maximum C:N ratio in topsoil (g/g)
! CNseq ..... C:N ratio (g/g) of the material immobilised
! fde ....... denitrification fraction (0<=fde<=1)
! modOrg .... protonity of organic acids:
!             1,2,3; 0=Oliver model; <0: not modelled
! pKpar() ... 1-3 parameters of organics model (meaning depends on INP%model)
! coacid() .. total concentration of organic acids (m*DOC) (mol/m3)
! temp() .... soil temperature (oC, average over 1T)
! ps() ...... precipitation surplus (runoff) (m/T)
! cmin%X . .. minimum [X] in soil leacheate (eq/m3) (X=NO3,Ca,Mg,K,PO4)
! Wea()%X ... weathering rate of X (eq/m3/T) (X=Ca,Mg,K,Na,PO4)
! Upt()%X ... net uptake of ion X (eq/m2/T) (X=NO3(+NH4),Ca,Mg,K,PO4)
! Dep()%X ... deposition of ion X (eq/m2/T) (X=SO4,NO3,NH4,Ca,Mg,K,Na,Cl)
! Nfix() .... fixation of N (eq/m2/T)
! OBSv() .... observations
! Mon ....... file for MONITOR
! Bal ....... file for mass and charge balances
!
! SMART|2 only:
! Cacarb0 ... INITIAL amount of carbonates in the soil (meq/kg)
! Alox0 ..... INITIAL amount of Al-(hydr)oxides (meq/kg)
! Padmax .... maximum PO4 adsorption capacity (meq/kg)
! Padh ...... half-saturation constant for PO4 sorption (eq/m3)
! expH ...... exponent of [H] in H-BC exchange (Gaines-Thomas only)
! pKAlpar() . pK-values for organic Al-complexation
```

```
! fni ....... nitrification fraction (0<=fni<=1)
! Alw() ..... weathering rate of Al (eq/m3/T)
!
! errbyte ... byte-vector for error messages
```

Readinpvsdp

```
! Reads input data for VSD+ from INP%file and, if not found, sets
! default values for some of them.
!
! INP
!  %model .... name of model ('VSD','SMART','SMART2')
!  %file ..... name of input data file
!  %path ..... path extracted from %file
!  %nvars .... number of keywords/variables incl. default ones
!  %key() .... keywords for variables
!  %line() ... lines with varaibles
!  %got() .... =.true., for those variables which were read from %file
!              or got default values
!  %def() .... =.true., if a default value has been set
!
! INPUT:
! IB ........ first index of time series vectors
! IE ........ last index of time series vectors
! iyrb ...... first year of simulation (integer)
! iyre ...... last year of simulation (integer)
! mstep ..... number of sub-periods within a year (integer)
!
! OUTPUT:
! CN() ...... C:N ratio of C pools (g/g)
! kni ....... maximum nitrification rate at Tref (yr-1)
! kde ....... maximum denitrification rate at Tref (yr-1)
! Clf() ..... amount of litterfall (g C/m2/yr)
! Nlf() ..... N content of litterfall (g N/m2/yr)
! QIlf() .... Quality index of litterfall (-)
! rfmi()..... reduction function of moisture, drought and temperature for mineralisation in RothC(-)
! rfni()..... reduction function of moisture, drought and temperature for nitrification (-)
! rfde()..... reduction function of moisture, drought and temperature for denitrification (-)
! fN2Oni .... N2O emissions as fraction of nitrification (-)
! fN2Ode .... N2O emissions as fraction of denitrification (-)
! Nfix() .... N fixation (eq/m2/yr)
! Nupeff .... uptake efficiency of available N (-)
! ctclay .... clay contents of the soil (%)
! Upt()%X ... net uptake of ion X (X=Ca, Mg, K) (eq/m2/T)
! errbyte ... byte-vector for error messages
```

VSDprep

```
! Assign/convert some variables:
!
! INPUT:
! expAl ........ exponent in [Al] = KAlox*[H]^expAl
! lgKAloxv() ... log10 of Al equilibrium constant ((eq/m3)^(1-expAl))
! modExc ....... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
! lgExcMat() ... 6x6 matrix of log10 of CatExc selectivity constants:
!                lgExcMat(i,j) for lgKij, i,j=H,Al,Ca,Mg,K,Na (Bc=Ca);
!                e.g. lgExcMat(1,3) = lgKHBc
! thick ........ soil thickness (m)
! EBc0 ......... initial base saturation (Ca+Mg+K)
! Dep0%X ....... deposition in first year (X=Ca,Mg,K)
! Wea0%X ....... weathering in first year (X=Ca,Mg,K)
! Upt0%X ....... uptake in first year (X=Ca,Mg,K)
!
! OUTPUT:
! ECa0 ......... initial exchangeable fraction of Ca; not changed if EBc0 < 0)
! EMg0 ......... initial exchangeable fraction of Mg; not changed if EBc0 < 0)
! EK0 .......... initial exchangeable fraction of K; not changed if EBc0 < 0)
! eqKv() ....... chemical (equilibrium) constants
!                %pCO2 .... partial CO2-pressure in soil solution (atm)
!                %Alox .... Al equilibrium constant ((eq/m3)^(1-expAl))
!                %expAl ... exponent in [Al]=eqK%Alox*[H]^expAl
! KAlBc ........ selectivity constant for Al-Bc exchange
! KHBc ......... selectivity constant for H-Bc exchange
```

VSDprun

```
! Runs the VSD+ model and returns results in aout().
!
! INPUT:
! IB ......... first index of time series vectors
! IE ......... last index of time series vectors
! NV ......... number of output/display variables
! iyrb ....... first year of simulation (iyrb >= IB)
! iyre ....... last year of simulation (iyre <= IE)
! eqKv() ..... chemical (equilibrium) constants
! thick ...... soil thickness (m)
! rho ........ bulk density (g/cm3)
! thetav() ... volumetric water content of the soil (m3/m3)
! CEC ........ cation exchange capacity of the soil (meq/kg)
! ECa ........ exchangeable fraction of Ca
! EMg ........ exchangeable fraction of Mg
! EK ......... exchangeable fraction of K
! parentCa ... if >=0 simulate calcareous soil; value of parentCa (<=1) is fraction of Ca
!              in limestone (rest is Mg, as e.g. in dolomite); if <0: non-calcareous soil
! ctclay ..... clay contents of the soil (%)
! modExc ..... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
! KAlBc ...... selectivity constant for Al-Bc exchange
! KHBc ....... selectivity constant for H-Bc exchange
! Cpool0 ..... initial amount of C in topsoil (g/m2)
! CNrat ...... C:N ratio in topsoil (g/g)
! temp() ..... annual average soil temperature (oC)
! ps() ....... precipitation surplus (runoff) (m/yr)
! coacid() ... total concentration of organic acids (m*DOC) (mol/m3)
! pKpar() .... 1-3 parameters of (Oliver-type) mono-protic organics model:
!              pK = par(21)+par(22)*pH-par(23)*pH^2
! Wea()%X .... weathering rate of X (X=Ca,Mg,K,Na,PO4) (eq/m3/yr)
! Upt()%X .... net uptake of X (X=NH4,NO3,Ca,Mg,K,PO4) (eq/m2/yr)
! Dep()%X .... deposition of ion X (eq/m2/yr);
!              X = SO4, NO3, NH4, Ca, Mg, K, Na, Cl, PO4
! kni ........ maximum nitrification rate at Tref (yr-1)
! kde ........ maximum denitrification rate at Tref (yr-1)
! CN() ....... C:N ratio of C pools (g/g)
! Nlf() ...... N litterfall (g N/m2/yr)
! Clf() ...... C litterfall (g C/m2/yr)
! QIlf() ..... Quality index of litterfall (-)
! rfmi() ..... reduction function for mineralisation (-)
! rfni() ..... reduction function for nitrification (-)
! rfde() ..... reduction function for denitrification (-)
! fN2Oni ..... N2O emissions as fraction of nitrification (-)
! fN2Ode ..... N2O emissions as fraction of denitrification (-)
! Nfix ....... N fixation (eq/m2/yr)
! Nupeff ..... uptake efficiency of available N (-)
! Sadmax ..... maximum SO4 adsorption capacity (meq/kg)
! Sadh ....... half-saturation constant for SO4 sorption (eq/m3)
! Padmax ..... maximum PO4 adsorption capacity (meq/kg)
! Padh ....... half-saturation constant for PO4 sorption (eq/m3)
! iss ........ option for desired sea-salt SO4:
!              =0: no sea-salt SO4 correction
!              =1: correct using Cl (i.e. Cl*=0)
!              =2: correct using Na (i.e. Na*=0)
! mdx ........ index function
!
! OUTPUT:
! aout(:,n) ... output time series for selected variable n
! errbyte ..... byte-vector for error messages
```

Seasalts

```
! For base cation and Cl depositions (given in eq in Dep), this subroutine
! returns their sea-salt fractions, assuming -- for iopt=1,2,3,4,5 -- that all
! Cl(iopt=1),Na,Mg,Ca,K(iopt=5) is sea-salt derived.
! [Seasalt-corrected depositions can then be computed as Dep* = Dep-Depss.]
! Also returned is an estimate of the sulfate originating from seasalts.
! Note: For inconsistent data Depss%SO4 can be < 0!
!
!
  integer,    intent(in)  :: iopt   ! option for which element is used to correct SO4dep (-)
  type(Ions), intent(in)  :: Dep    ! deposition of ion X (eq/m2/yr);
!                                     X = SO4, NO3, NH4, Ca, Mg, K, Na, Cl, PO4
  type(Ions), intent(out) :: Depss  ! sea-salt derived deposition of ion X (eq/m2/yr)
```

VSDp

```
! Very Simple Dynamic plus (VSD+) [soil acidification] model:
! Calculates for a single time step a number of soil chemical
! parameters depending on element inputs and chemical soil status.
!
! INPUT:
! start ..... start flag; if true: initialise certain variables for
!             use in simulation; set to false afterwards (see NOTES)
! eqK ....... chemical (equilibrium) constants
!             %pCO2 .... partial CO2-pressure in soil solution (atm)
!             %HCO3 .... bi-carbonate equilibrium constant (mol/m3)^2/atm
!             %Alox .... Al equilibrium constant ((eq/m3)^(1-expAl))
!             %expAl ... exponent in [Al]=eqK%Alox*[H]^expAl
! thick ..... soil thickness (m)
! rho ....... bulk density (g/cm3)
! theta ..... volumetric water content of the soil (m3/m3)
! thetao .... volumetric water content of the soil at previous timestep (m3/m3)
! CEC ....... cation exchange capacity of the soil (meq/kg)
! Sadmax .... maximum SO4 adsorption capacity (meq/kg)
! Sadh ...... half-saturation constant for SO4 sorption (eq/m3)
! Padmax .... maximum PO4 adsorption capacity (meq/kg)
! Padh ...... half-saturation constant for PO4 sorption (eq/m3)
! parentCa .. if >=0 simulate calcareous soil; value of parentCa (<=1) is fraction of Ca
!             in limestone (rest is Mg, as e.g. in dolomite); if <0: non-calcareous soil
! ctclay .... clay contents of the soil (%)
! modExc .... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
! KAlBc ..... selectivity constant for Al-Bc exchange
! KHBc ...... selectivity constant for H-Bc exchange
! temp ...... annual average soil temperature (oC)
! ps ........ precipitation surplus (m/yr)
! coacid .... total concentration of organic acids (m*DOC) (mol/m3)
! pKpar() ... 1-3 parameters of (Oliver-type) mono-protic organics model:
!             pK = pKpar(1)+pKpar(2)*pH-pKpar(3)*pH^2
! Wea%X ..... weathering rate of X (X=Ca,Mg,K,Na) (eq/m3/yr)
! Upt%X ..... net uptake of X (X=NO3+NH4,Ca,Mg,K) (eq/m2/yr)   note: output for NO3 and NH4
! Dep%X ..... deposition of X (X=SO4,NO3+NH4,Ca,Mg,K,Na,Cl) (eq/m2/yr)
! CN() ...... C:N ratio of C pools (g/g)
! Nlf ....... N litterfall (g N/m2/yr)
! Clf ....... C litterfall (g C/m2/yr)
! QIlf ...... Quality index of litterfall (-)
! rfmi ...... reduction function of moisture, drought and temperature for mineralisation (-)
! rfni ...... reduction function of moisture, drought and temperature for nitrification (-)
! rfde ...... reduction function of moisture, drought and temperature for denitrification (-)
! kni ....... maximum nitrification rate at Tref (yr-1)
! kde ....... maximum denitrification rate at Tref (yr-1)
! fN2Oni .... N2O emissions as fraction of nitrification (-)
! fN2Ode .... N2O emissions as fraction of denitrification (-)
! Nfix ...... N fixation (eq/m2/yr)
! Nup ....... total uptake of N (eq/m2/yr)
! Nupeff .... uptake efficiency of available N (-)
!
! OUTPUT:
! CNrat ..... C:N ratio in topsoil (g/g)
! Nim ....... N immobilized (eq/m2/yr)
! Nde ....... N denitrified (eq/m2/yr)
! cH ........ H+ concentration (eq/m3)
! Conc%X* ... concentration of ion X (SO4,NO3,NH4,Ca,Na,Cl) (eq/m3);
!             if Gapon: Conc%Ca=[Ca]+[Mg]+[K], Conc%Mg=Conc%K=0
! cAl ....... aluminium concentration (eq/m3)
! cOrg ...... concentration of organic anions (eq/m3)
! cHCO3 ..... bicarbonate concentration (eq/m3)
! cANC ...... ANC concentration (as function of [H]) (eq/m3)
! ECa* ...... exchangeable fraction of Ca [ECa=ECa+EMg+EK in case of Gapon]
! EMg* ...... exchangeable fraction of Mg [EMg = 0 in case of Gapon]
! EK* ....... exchangeable fraction of K  [EK = 0 in case of Gapon]
! EAl ....... exchangeable fraction of Al
! EH ........ exchangeable fraction of H (ECa+EMg+EK+EAl+EH=1)
! errbyte ... byte-vector holding (error) messages:
!             if char(errbyte(1)) not blank, there IS an (error)message!
! Cpool%Cfr . size of C pools (Cfr=fe,fs,mb,hu) (g/m2)
! Nni ....... N nitrified (eq/m2/yr)
! N2Oem ..... N2O emissions (mol N/m2/yr)
!
! NOTES:
! +These variables have to hold the values from the previous timestep;
!  i.e. at the first call they have to be the initial values.
! *These variables have to hold the values from the previous timestep, UNLESS
!  start=.true.: then they are initialized with equilibrium values (ECa,EMg,EK only if ECa<0).
```

CNorg

```
! v1.0 created: 14/07/2008, L. Bonten
! cosmetic changes: 02/08/2012, M. Posch
! v 2.0 based on RothC: 1/11/2013, L. Bonten
!
! Updates C pools for a single time step.
! Also calculates N immobilisation/mineralisation.
!
! INPUT:
! start ..... start flag; if true: initialise C pools
! Dep%X ..... deposition (X=NH4,NO3) (eq/m2/yr)
! Diss%X .... amount of ion X in solution(X=NO3,NH4) (eq/m2);
! CN() ...... C:N ratio of C pools (g/g)
! Clf ....... C litterfall (g C/m2/yr)
! Nlf ....... N litterfall (g N/m2/yr)
! QIlf ...... Quality index of litterfall (-)
! rfmi ...... reduction function of moisture, drought and temperature for mineralisation (-)
! Nfix ...... biological N fixation (eq/m2/yr)
! Nup ....... uptake of total N (eq/m2/yr)
! Nupeff .... fraction of available N that plants can uptake (-)
! ctclay .... clay contents of the soil (%)
!
! OUTPUT:
! Nim ....... net N immobilisation (mineralisation if <0) (eq/m2/yr)
! Cpool() ... size of C pools (g/m2);
!             (has to hold values from previous time step; if start=.true. only sum counts)
! Upt%X ..... uptake of X (X=NO3,NH4) (eq/m2/yr)
! CNrat ..... overall C:N ratio (g/g) (input when start=.true.)
! errsmg .... error message
```

VSDcore

```
! Very Simple Dynamic (VSD) [soil acidification] model:
! Calculates for a single time step a number of soil chemical parameters
! depending on element inputs and soil chemical status.
!
! INPUT:
! start ...... start flag; if true: initialise certain variables for
!              use in simulation; set to false afterwards (see NOTES)
! parentCa ... if >=0 simulate calcareous soil; value of parentCa (<=1) is fraction of Ca
!              in limestone (rest is Mg, as e.g. in dolomite); if <0: non-calcareous soil
! eqK ........ chemical (equilibrium) constants
!              %pCO2 .... partial CO2-pressure in soil solution (atm)
!              %Alox .... Al equilibrium constant ((eq/m3)^(1-expAl))
!              %expAl ... exponent in [Al]=eqK%Alox*[H]^expAl
! thick ...... soil thickness (m)
! rho ........ bulk density (g/cm3)
! theta ...... volumetric water content of the soil (m3/m3)
! thetao ..... volumetric water content of the soil at previous timestep (m3/m3)
! CEC ........ cation exchange capacity of the soil (meq/kg)
! Sadmax ..... maximum SO4 adsorption capacity (meq/kg) (0=no S-sorption)
! Sadh ....... half-saturation constant for SO4 sorption (eq/m3)
! Padmax ..... maximum PO4 adsorption capacity (meq/kg) (0=no P-sorption)
! Padh ....... half-saturation constant for PO4 sorption (eq/m3)
! modExc ..... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
! KAlBc ...... selectivity constant for Al-Bc exchange
! KHBc ....... selectivity constant for H-Bc exchange
! coacid ..... total concentration of organic acids (m*DOC) (mol/m3)
! pKpar() .... 1-3 parameters of (Oliver-type) mono-protic organics model:
!              pK = pKpar(1)+pKpar(2)*pH-pKpar(3)*pH^2
! temp ....... annual average soil temperature (oC)
! ps ......... precipitation surplus (m/a)
! Influx%X ... Net input flux of ion X (eq/m2/T) (X=SO4,NO3,NH4,Ca,Mg,K,Na,Cl,PO4)
!
! OUTPUT:
! cH ......... H+ concentration (eq/m3)
! Conc%X* .... concentration of ion X (X=SO4,NO3,NH4,Ca,Mg,K,Na,Cl) (eq/m3);
!              [Gapon: only Conc%Ca+Conc%Mg+Conc%K makes sense]
! cAl ........ aluminium concentration (eq/m3)
! cOrg ....... concentration of organic anions (eq/m3)
! cHCO3 ...... bicarbonate concentration (eq/m3)
! cANC ....... ANC concentration (as function of [H]) (eq/m3)
! Solid%X* ... amount of solid (sorbed) X (meq/kg) (X=SO4)
! ECa* ....... exchangeable fraction of Ca [ECa=ECa+EMg+EK in case of Gapon]
! EMg* ....... exchangeable fraction of Mg [EMg = 0 in case of Gapon]
! EK* ........ exchangeable fraction of K  [-"-]
```

```
! EAl ........ exchangeable fraction of Al
! EH ......... exchangeable fraction of H (ECa+EMg+EK+EAl+EH=1)
! errbyte .... byte-vector holding (error) messages:
!               if char(errbyte(1)) not blank, there IS an (error)message!
!
! NOTES:
! *These variables have to hold the values from the previous timestep,
!  UNLESS start=.true.: then they are initialized with equilibrium values
!                       (ECa,EMg,EK only if ECa<0).
```

VSDpSMB

```
!
! Computes critical loads (CLF) of acidity and nutrient N for selected criteria with the SMB model.
! Note: critical loads for acidity only for non-calcareous soils
!
! INPUT:
! iCrit ...... option for computing CLmaxS, CLminN and CLmaxN:
!              =1: CritLim = molar [Al]:[Bc]
!              =2: CritLim = [Al] (eq/m3)
!              =3: CritLim = EBc (base saturation) (fraction, NOT%)
!              =4: CritLim = pH
!              =5: CritLim = [ANC] (eq/m3)
!              =6: CritLim = molar [Bc]:[H] ([Al]=0 => not compatible with VSD!)
!              =7: CritLim = Alw ! no Al depletion
!              =8: CritLim = molar [Al]:[Ca]
!              =9: CritLim = [Al]:[Bc], only if [Al]>0.1
!              =10:CritLim = [NO3]+[NH4] (eq/m3)
!              =11:CritLim = Navail (eq/m2/yr)
!              not used: =12:CritLim = C:N ratio (g/g)
! CritLim ... see iCrit above.
! eqK ....... chemical (equilibrium) constants
! thick ..... soil thickness (m)
! modExc .... cation exchange model option: 1=Gaines-Thomas, 2=Gapon
! KAlBc ..... selectivity constant for Al-Bc exchange
! KHBc ...... selectivity constant for H-Bc exchange
! parentCa .. if >=0 simulate calcareous soil; value of parentCa (<=1) is fraction of Ca
!             in limestone (rest is Mg, as e.g. in dolomite); if <0: non-calcareous soil
! temp ...... annual average soil temperature (oC)
! ps ........ precipitation surplus (m/a)
! coacid .... total concentration of organic acids (m*DOC) (mol/m3)
! pKpar() ... 1-3 parameters of (Oliver-type) mono-protic organics model:
!             pK = pKpar(1)+pKpar(2)*pH-pKpar(3)*pH^2
! Wea%X ..... weathering rate of X (X=Ca,Mg,K,Na) (eq/m3/a)
! Upt%X ..... net uptake of X (X=Ca,Mg,K) (eq/m2/a)
! Dep%X ..... deposition of X (X=Ca,Mg,K,Na,Cl) (eq/m2/a)
! kni ....... maximum nitrification rate at Tref (yr-1)
! kde ....... maximum denitrification rate at Tref (yr-1)
! rfni ...... reduction function of moisture, drought and temperature for nitrification (-)
! rfde ,..... reduction function of moisture, drought and temperature for denitrification (-)
! Nfix ...... N fixation (eq/m2/yr)
! Nup ....... N uptake (eq/m2/yr)
! Nlf ....... N in litterfall (g/m2/yr)
! gridsize .. defines number of nodes for drawing CL function (nodes = (gridsize+1)^2 )
!
! IN/OUTPUT:
! limitS .... maximum S deposition for drawing CL function
! limitN .... maximum N deposition for drawing CL function
!
! OUTPUT:
! ANCle ..... critical ANC leaching (eq/m2/a)
! CLx() ..... critical limits, x-axis in CL function; 0-gridsize
! CLy() ..... critical limits, y-axis in CL function; 0-gridsize
! CLz() ..... critical limits, z-axis in CL function; 0-(gridsize+1)^2-1
! CLmaxS .... maximum critical load of S (eq/m2/a)
! CLminN .... minimum critical load of N (eq/m2/a)
! CLmaxNO ... maximum critical load of NO (eq/m2/a); is -99 if complete denitrification
! CLmaxNH ... maximum critical load of NH3 (eq/m2/a); is -99 if no maximum critical load
! errbyte ... byte-vector for error messages
```

Annex 2 Monitor

Monitor

A subroutine for monitoring model output

Description & User Manual

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Introduction

This manual describes the use of the subroutine *Monitor*. This subroutine, which can be called from any Fortran program, produces a PostScript file of up to 9 graphs each in maximal 25 frames of user-selected variables (time series) of a model run. In addition, it can produce an ASCII file containing the values of the selected variables.
This manual consists of two parts: Part A is for users who have an executable program which calls *Monitor*. It explains the parameters in the file that control the output of *Monitor*. For users, who are in the position to link the subroutine *Monitor* to a Fortran program of their choice, Part B explains how to do that.

Part A: Running programs with built-in *Monitor*

A program calling *Monitor* requires also a parameter-file, which tells *Monitor* what to plot and/or write. The name of that parameter-file is passed to the subroutine *Monitor* in its argument list, and thus the user can change its name only if s/he can also change that argument.

Each line in a parameter file starts with the fixed name (keyword) of a parameter, followed by the parameter value(s), separated from the keyword by blank(s). The order of parameters (=lines) is arbitrary. In addition, there can be comment lines, i.e. lines starting with an exclamation mark ('!'), anywhere in the file – they are ignored by *Monitor*. The meaning of the parameters and their allowed values are explained below. An example of a parameter file is given at the end of Part A.

Parameters

In this section the parameters and their allowed values, making up a parameter file, are described. Every parameter name (keyword) is listed in ***bold italics***, followed by an explanation. Symbols enclosed between <…> next to a keyword (and separated by '|') have the following meaning:
(a) ? ... a question mark as parameter value means that its value(s) are asked interactively;
(b) *n* … maximum number of entries of that keyword
(c) Y/n … the (only) valid value for this variable is 'y' or 'n' (standing for 'yes' and 'no', resp.). A capital 'Y' means that 'yes' is the default, and this is only overruled if the variable is set to 'n' (and vice versa for y/N); 'Y' and 'N' are interpreted as 'y' and 'n', resp.

In character strings to be displayed as text in the PostScript output (e.g., the variable *title*) sub- and superscripts can be obtained by prefixing them in the string with '_' and '^', resp., and ending with a blank. E.g., 'mol_c ha^–1 yr^–1' produces 'mol$_c$ha^{-1}yr^{-1}'.

NOTE: Unless it starts with '\' or 'X:' (X=drive letter), it is assumed that the path of a file (*outfile*, *PSfile*, *compfile*) is to be taken from the directory of this file.

outfile <?>
Name of ASCII file to which the displayed data are written. With an optional suffix '/p' ('plain') to the filename all comment lines except the last (i.e. the column headers) on top of the file are suppressed. The shape of such an output file is described below.
If absent or blank, no output file is produced.

The first line in an *outfile* is a comment line (i.e. starts with '!'), with the ***title*** (see below) numerical codes that indicate which variables are written to the file. This is followed by *nvar* (=number of variables to be written out) comment lines, giving the (short, internal) name of the variable (one per line) and 'explaining' it (full name, units). The last commented line is of the form '`!count,time,Var1,Var2,…`'.
After that, 2+*nvar* columns of data are written in the user-defined (see below) or in default format. Column 1 contains the step number (counter), always starting at 0, column 2 contains the 'year', each repeated as many times as there are subdivisions of the 'year' in the simulation. Columns 3 to 2+*nvar* contain the values of the variables (in the order selected by the user). The 'i'(=integral) in front of a variable number (see below) has no influence on the writing (it's only for the graph). The first lines written to an *outfile* could look like this:

```
!VSD-Test
!Sdep : S deposition (eq/m2/a)
!Ndep : N deposition (eq/m2/a)
!Cpool : C pool (g/m2)
!bsat : EBc
!pH : pH
!cANC : [ANC] (eq/m3)
!AlBc : [Al]/[Ca+Mg+K] (mol/mol)
!balance : Soil charge balance
!count,time,Sdep,Ndep,Cpool,bsat,pH,cANC,AlBc,balance
0 1900.5 0.100 0.030 4000.000 0.377 4.073 -0.250 1.032 0.000
1 1901.5 0.103 0.031 4000.000 0.377 4.070 -0.255 1.040 0.000
2 1902.5 0.106 0.032 4000.000 0.377 4.066 -0.261 1.050 0.000
3 1903.5 0.109 0.033 4000.000 0.377 4.061 -0.269 1.062 0.000
.....
```

fmtout
Fortran format (incl. brackets) for data in *outfile*; not read if no *outfile*.
Default='(i6,99g13.5)'.

PSfile <?>
Name of PostScript (EPS) file (max. 128 characters). If no extension is given, '.eps' is appended by *Monitor*. If absent or blank, no PostScript file is produced.

NOTE: If neither *outfile* nor *PSfile* is specified, *Monitor* does nothing. This allows to 'switch of' (i.e. not to use) *Monitor*, even when it is linked to a program.

postview
A program (executable incl. path) to post-process (display) the PostScript file. After the PostScript file is created, this program is invoked by *call system* (*'postview PSfile'*).
If absent or no *PSfile*, not executed.

varlist <?>
ID-numbers of the variables selected for display and/or writing. It is possible to display up to 9 variables in one frame/pane by linking them with a '&'-sign. If a variable is preceded by an 'i' (for **i**ntegrate), the running sum ('integral') of that variable is displayed; that sum is reset to zero after *iperiod* steps (see below). The variables are displayed in the order in which they are selected. Up to 25 frames can be drawn. If more than 25 frames or more than 9 variables per frame are selected, *Monitor* stops with an error message.
If absent or blank, *Monitor* does nothing!

Compfile <?|9>
Name of file with output of a previous run (for visual comparison). The file has to be in the form of an *outfile* (see above). The last commented line tells *Monitor* which variables there are; and graphs of those variables, if they are chosen in the current model run, are plotted in the respective frames as black dashed lines. If there is more than one *compfile*, they are processed in the order given.
If blank or missing, no comparisons are plotted.

title <?>
Text (max. 127 chars) written as title to the graphical output; also written as first commented line to *outfile*, if it does not have the '/p' clause.
If absent, `Infobyte` from the argument list of *Monitor* (see Part B) is written as title.

author
Text (max. 127 chars) written in small letters in the upper-left corner of the display area.
If absent, no *author*.

date
Date and time is written in small letters in upper-right corner of the display area, defined as an integer: 0=No (default); 1=yes.

canvasxy
x:y ratio of overall graphical output window ('canvas').
Default: *canvasxy*=1.25
NOTE: The following variables apply to all windows/graphs.

layers
ID-numbers of layers to be plotted …
Default: *layers*=1.

xmin <?>
Minimum value of the time series ('year') to be displayed in every graphical window and/or written out. Together with *xmax* (see below) these parameters (if they define a meaningful interval), overrule the values min- and max-values from the argument list of *Monitor* (thus allowing to display only parts of a simulation).

Default: `iyrb`-value from the argument list of *Monitor*.

xmax <?>
Maximum value of the time series ('year') to be displayed in every graphical window and/or written out (see *xmin*).
Default: `iyre`-value from the argument list of *Monitor*.

intx <?>
1–3 integers:
First: Number of intervals to be marked with vertical lines in the graphical windows; also controls the labelling of the horizontal axes.
Second: Step size for labelling; e.g. step=2 means every second label is left out (optional).
Third: Number of labels skipped in the beginning (optional).
Default: 2 1 0.

gridgray
Grayshade (integer: black=0–255=white) of x-y grid lines in all windows/panes.
Default: *gridgray*=200.

labx <Y/n>
Label x-axes of lower-most panes?

formatx
Fortran format (incl. brackets) for labelling the horizontal axes.
If absent, determined by *Monitor*.

xskip
Number of 'years' after *xmin* that are ***not*** displayed on the screen and/or written to a file. If, as a consequence, the number of steps to be displayed is less than two, the program terminates with an error message.
Default: *xskip*=0.

xvert
A vertical line is drawn at this x-value in every display window (if within).
If absent, no vertical lines are drawn.

yzero
If *yzero* ≥ 0, a horizontal black line of thickness *yzero* is drawn at y=0 if $y_{min}<0$ and $y_{max}>0$.

iperiod
After each step, which is a multiple of this integer, the summation ('integration') of variables (i.e. those preceded by an 'i', see *varlist*) is restarted from zero.
If absent, *iperiod* is set to a very large number.

statist
Integer controlling the calculation of a 'statistic' of the displayed variables.
If > 0, the sum of the displayed values for each variable is divided by *statist* at the last call to *monitor* and written in the upper-right corner of the window/pane for that variable (e.g., *statist*=1 => the sum for each variable is shown).
If = 0, the arithmetic mean for each variable is shown.
If = –1, the last value for each variable is shown.
Default: no *statist*-ic.

lthick
Thickness of the lines in the graphs (also comparison graphs):
=0: thinnest line (1/600 inch); =2: fairly thick line.
Default=1.

colors
Integers (black=0–555=white; see Figure A2.1) defining the colours of the graphs: 1st colour for 1st line in every window, etc. A maximum of 9 values is read.
If an integer is 100**R*+10**G*+*B*, then the corresponding 8-bit code of the red, green and blue component is 51**R*, 51**G* and 51**B*, resp.
If absent, default colours are used (red, green, blue, …)

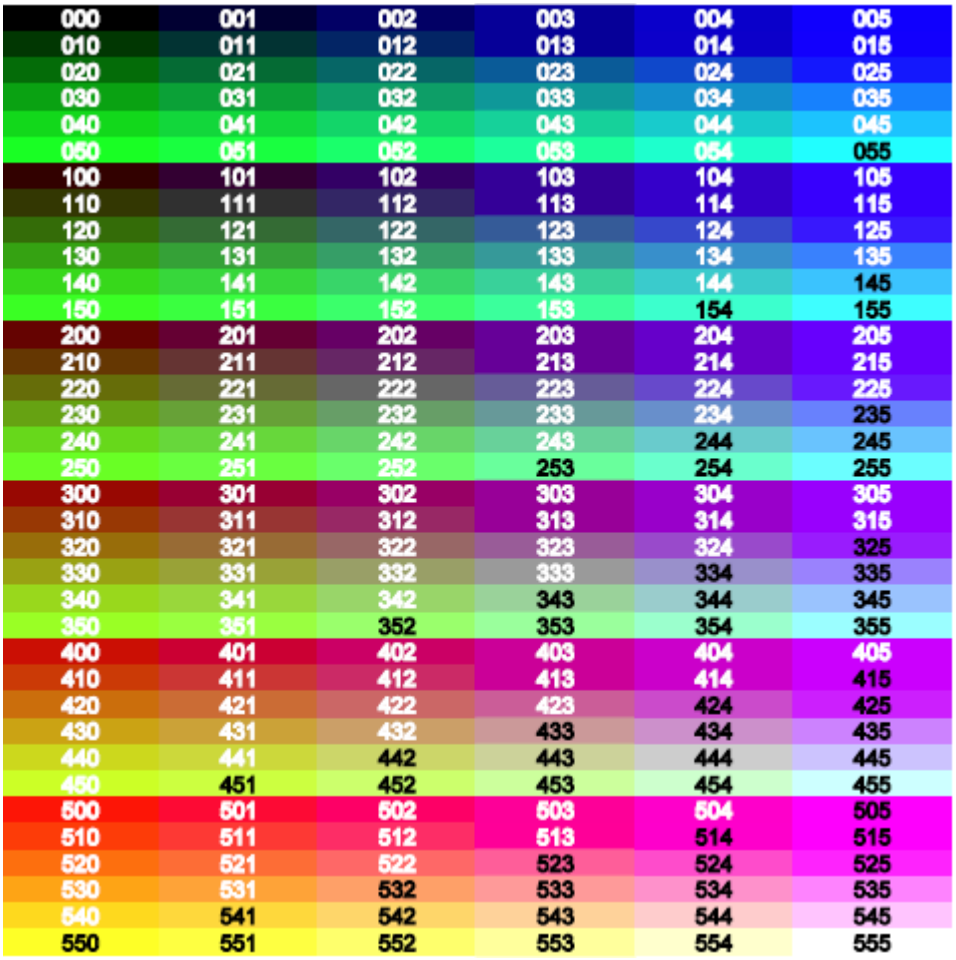


Figure A2.1*: Colours as defined by colors. Note that the 'true' colours depend on the (type of) printer.*

During execution

During running a program that calls *Monitor*, the interactive input depends on the parameter file (see above).

For every line in the parameter-file containing a single question mark ('?') as allowed input, *Monitor* will ask for the filename/string interactively, and this string is remembered in subsequent calls [between square brackets]. In order to invoke the same string, press ENTER.

In case of an interactive input of the variables (see *varlist*), the user is prompted with the list of variables which can be displayed and/or printed by *Monitor*. The user can select variables by typing their numbers (they don't have to be in ascending order and they can be repeated). If an invalid (too large) variable number is selected, *Monitor* prints a warning message and asks for another choice. If there are more than 50 display variables to choose from, they are listed in "batches" of (maximal) 50 variables each. Numbers of variables chosen are remembered in subsequent calls [between square brackets]. In order to plot/print the remembered variables, just press ENTER. If you want to *add* numbers of variables already chosen (=remembered), the first (non-blank) character of the additional choices has to be a 'u' (for **u**nion). If you are happy with your (previous) choice of variables and want to prevent display of further screens (in case of many variables), type 'q' (for **q**uit). Up to 9 variables can be displayed in one window on the screen by linking their numbers with

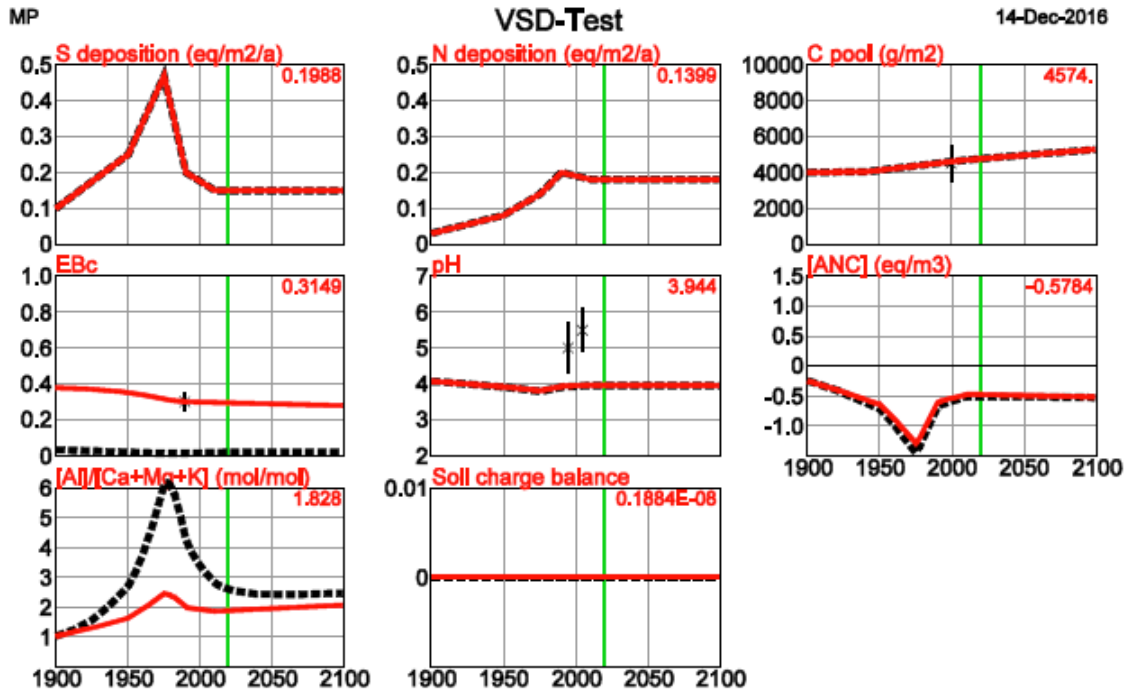
the '&'-sign. If a variable is preceded by an 'i' (for **i**ntegrate), the running sum ('integral') of that variable is displayed; it is reset to zero after every multiple of *iperiod* steps (see above).

Example:

An example of a *Monitor* parameter file could look like this:

```
outfile vsd.out
fmtout (i3,f7.1,99f9.3)
PSfile vsd.eps
Y_change cANC; '[ANC] (eq/m3)'; -1.5 1.5 6
Y_change AlBc; '[Al]/[Ca+Mg+K] (mol/mol)'; 0 6 6
varlist 3 4 12 26 32 45 46 51
compfile vsd1.out
title VSD-Test
author MP
date 1
canvasxy 1.2
intx 4
xvert 2020
yzero 0.5
statist 0
lthick 2
gridgray 153
```

A sample plot of a PostScript file, generated by *Monitor*, is shown for illustration:



Part B: Calling *Monitor* from a Fortran program

Here we describe how the subroutine *Monitor* is called from a Fortran program. A typical program fragment could look like this:

```
.....
integer, parameter :: mstep=1, MXL=1 ! yearly time step and single layer
integer, parameter :: IB=1800, IE=3000, NYRS=(IE-IB+1)*mstep
integer, parameter :: NV=90 ! max. number of output variables
!
byte :: Infobyte(128)
character(len=128) :: monfil
integer :: j, iyrb, iyre, ntime
real :: areac, tv(NYRS), aout(NYRS,NV)
type(datafile) :: OBSv(NV)
!
.....
ntime = 1
do iyr = iyrb,iyre
do m = 1,mstep
ntime = ntime+1
.....
call model (...,aout(ntime,:))
.....
end do
end do
.....
areac = 0
forall (j=1:ntime) tv(j) = iyrb+j-0.5
!
call Monitor (monfil,areac,Infobyte,IB,IE,iyrb,iyre,mstep,MXL,ntime, &
& tv,aout,OBSv)
.....
```

The arguments of *Monitor* have the following meaning: The character string `monfil` is the name of the parameter file that determines which variables should be displayed, and how (see Part A). The real parameter `areac` should be set to zero (for the VSD+model). `Infobyte` holds a character string as byte-vector put as title above the graphs and in the output file. However, it is overwritten by the *title*-variable in `monfil` if that is specified (see Part A). The integers `IB` and `IE` determine the maximum time window (in years) within which simulations can be carried out. The integer variables `iyrb`, `iyre` and `mstep` determine the time period of the simulation (`iyre-iyrb+1` 'years' with `mstep` 'months' each) and the (default) window to be displayed during the model run. The integer variable `ntime` is the number of time steps (`ntime=(iyre-iyrb+1)*mstep`). The real vector `tv` holds the values on the x-axes at which the output value should be plotted, e.g. at the middle of the interval representing the modelling time step. The real array `aout` holds the values of all variables that can be displayed (`aout(:,n)` holds the time series of variable `n`). Finally, the variable `OBSv` is a vector of type 'datafile' holding all necessary information on the 'observations' to be plotted in addition to the model output. The Fortran type 'datafile' is defined as:

```
type datafile
logical :: there
character(len=256) :: file
character(len=64) :: fmt
character(len=1) :: style
integer :: ncol, ipar(9)
real :: scal, par(9)
end type datafile
```

Before running a program calling *Monitor* a parameter-file which tells *Monitor* what to plot and/or write has to be prepared. The name of this file is arbitrary, and it is passed to *Monitor* in its argument list (monfil). For description of its contents and an example of such a file see Part A.

Annex 3 Tests VSD+

1. Computed pH from the charge balance (eq. 1), for the Gapon

input file: vdp_1.in

output file: vsdp_1.out

```
!cH       : [H+] (eq/m3)
!cSO4     : [SO4--] (eq/m3)
!cNO3     : [NO3-] (eq/m3)
!cNH4     : [NH4+] (eq/m3)
!cBc      : [Ca+Mg+K] (eq/m3)
!cNa      : [Na] (eq/m3)
!cCl      : [Cl] (eq/m3)
!cAl      : [Al3+] (eq/m3)
!cOrg     : [Org-] (eq/m3)
!cHCO3    : [HCO3-] (eq/m3)
```

!count	,time	,cH	,cSO4	,cNO3	,cNH4	,cBc	,cNa	,cCl	,cAl	,cOrg	,cHCO3	anions	cations	H+ from charge balance (eq 1)	check
0	1960.5	0.14202	0.5	0.98659	1.95E-02	0.47	0.33333	0.33333	0.85937	2.51E-03	1.79E-03	1.824221	1.68E+00	0.14202	1.000
1	1961.5	0.13914	0.5	0.91236	1.26E-02	0.45687	0.33333	0.33333	0.80811	2.52E-03	1.83E-03	1.750038	1.61E+00	0.13914	1.000
2	1962.5	0.13816	0.5	0.89254	1.26E-02	0.45505	0.33333	0.33333	0.79109	2.52E-03	1.84E-03	1.730235	1.59E+00	0.13816	1.000
3	1963.5	0.13796	0.5	0.89095	1.27E-02	0.45703	0.33333	0.33333	0.78766	2.52E-03	1.85E-03	1.728648	1.59E+00	0.13795	1.000
4	1964.5	0.13802	0.5	0.89489	1.28E-02	0.45967	0.33333	0.33333	0.78879	2.52E-03	1.85E-03	1.732587	1.59E+00	0.13803	1.000
5	1965.5	0.13819	0.5	0.90056	1.29E-02	0.46214	0.33333	0.33333	0.79173	2.52E-03	1.84E-03	1.738254	1.60E+00	0.13819	1.000
6	1966.5	0.13842	0.5	0.90684	1.30E-02	0.46423	0.33333	0.33333	0.7956	2.52E-03	1.84E-03	1.744530	1.61E+00	0.13842	1.000
7	1967.5	0.13868	0.5	0.91338	1.30E-02	0.46596	0.33333	0.33333	0.80005	2.52E-03	1.84E-03	1.751066	1.61E+00	0.13868	1.000
8	1968.5	0.13896	0.5	0.92006	1.31E-02	0.46736	0.33333	0.33333	0.80494	2.52E-03	1.83E-03	1.757741	1.62E+00	0.13897	1.000
9	1969.5	0.13926	0.5	0.92683	1.32E-02	0.4685	0.33333	0.33333	0.81017	2.52E-03	1.83E-03	1.764506	1.63E+00	0.13926	1.000
10	1970.5	0.13957	0.5	0.93367	1.33E-02	0.46942	0.33333	0.33333	0.81568	2.51E-03	1.83E-03	1.771341	1.63E+00	0.13957	1.000

2: Computed pH from the charge balance (eq. 1), for the Gaines Thomas exchange

input file: vdp_1_gt.in output file: vsdp_1_gt.out

```
!cH       : [H+] (eq/m3)
!cSO4     : [SO4--] (eq/m3)
!cNO3     : [NO3-] (eq/m3)
!cNH4     : [NH4+] (eq/m3)
!cBc      : [Ca+Mg+K] (eq/m3)
!cCa      : [Ca] (eq/m3)
!cMg      : [Mg] (eq/m3)
!cK       : [K] (eq/m3)
!cNa      : [Na] (eq/m3)
!cCl      : [Cl] (eq/m3)
!cAl      : [Al3+] (eq/m3)
!cOrg     : [Org-] (eq/m3)
!cHCO3    : [HCO3-] (eq/m3)
```

!count	,time	,cH	,cSO4	,cNO3	,cNH4	,cBc	,cCa	,cMg	,cK	,cNa	,cCl	,cAl	,cOrg	,cHCO3	anions	cations	H+ from charge balance (eq 1)	check
0	1960.5	0.14202	0.5	0.98659	1.95E-02	0.470000	0.003333	0.266670	0.200000	0.333330	0.333330	0.859370	0.002506	0.001795	1.824221	1.68E+00	0.14202	1.000
1	1961.5	0.139	0.5	0.91236	1.26E-02	0.459370	0.002035	0.261330	0.196000	0.333330	0.333330	0.805750	0.002517	0.001834	1.750040	1.61E+00	0.13901	1.000
2	1962.5	0.13795	0.5	0.89252	1.26E-02	0.458730	0.001274	0.261400	0.196050	0.333330	0.333330	0.787600	0.002521	0.001847	1.730218	1.59E+00	0.13796	1.000
3	1963.5	0.13774	0.5	0.89092	1.27E-02	0.460950	0.000806	0.262940	0.197210	0.333330	0.333330	0.783920	0.002522	0.001850	1.728622	1.59E+00	0.13774	1.000
4	1964.5	0.13782	0.5	0.89485	1.28E-02	0.463310	0.000511	0.264460	0.198340	0.333330	0.333330	0.785320	0.002521	0.001849	1.732550	1.59E+00	0.13782	1.000
5	1965.5	0.13802	0.5	0.90052	1.29E-02	0.465200	0.000324	0.265640	0.199230	0.333330	0.333330	0.788800	0.002520	0.001847	1.738217	1.60E+00	0.13803	1.000
6	1966.5	0.13829	0.5	0.9068	1.30E-02	0.466590	0.000206	0.266510	0.199880	0.333330	0.333330	0.793340	0.002520	0.001843	1.744493	1.61E+00	0.13827	1.000
7	1967.5	0.13859	0.5	0.91335	1.30E-02	0.467580	0.000130	0.267120	0.200340	0.333330	0.333330	0.798490	0.002518	0.001839	1.751037	1.61E+00	0.13858	1.000
8	1968.5	0.13891	0.5	0.92004	1.31E-02	0.468280	0.000083	0.267540	0.200660	0.333330	0.333330	0.804060	0.002517	0.001835	1.757722	1.62E+00	0.13890	1.000
9	1969.5	0.13924	0.5	0.92682	1.32E-02	0.468760	0.000052	0.267830	0.200870	0.333330	0.333330	0.809920	0.002516	0.001830	1.764496	1.63E+00	0.13925	1.000
10	1970.5	0.13959	0.5	0.93366	1.33E-02	0.469090	0.000033	0.268030	0.201020	0.333330	0.333330	0.815980	0.002515	0.001826	1.771331	1.63E+00	0.13959	1.000

3. Concentration of an ion that is a tracer (eq. 2); used [SO_4^{2-}] to test, using a sudden decrease in input halfway the simulation period

```
input file: vdp_2.in, output file vsdp_2.out
!cH      : [H+] (eq/m3)
!cSO4    : [SO4--] (eq/m3)
!ps      : Precipitation surplus (m/yr)
!Sdep    : S deposition (eq/m2/yr)
```

thick	0.5
theta	0.25
fcap	0.125

!count	,	time	,cH	,cSO4	,ps	,Sdep	to compute concentrations: eq 2 for cSO4 using eqA8 to solve	check
	0	1960.5	0.16286	0.5	0.3	0.15		
	1	1961.5	0.16038	0.5	0.3	0.15	0.50000	1.000
	2	1962.5	0.15969	0.5	0.3	0.15	0.50000	1.000
	3	1963.5	0.15969	0.5	0.3	0.15	0.50000	1.000
	4	1964.5	0.15989	0.5	0.3	0.15	0.50000	1.000
	5	1965.5	0.16014	0.5	0.3	0.15	0.50000	1.000
	6	1966.5	0.16041	0.5	0.3	0.15	0.50000	1.000
	7	1967.5	0.16068	0.5	0.3	0.15	0.50000	1.000
	8	1968.5	0.16096	0.5	0.3	0.15	0.50000	1.000
	9	1969.5	0.16124	0.5	0.3	0.15	0.50000	1.000
	10	1970.5	0.16151	0.5	0.3	0.15	0.50000	1.000
	11	1971.5	0.16179	0.5	0.3	0.15	0.50000	1.000
	12	1972.5	0.16207	0.5	0.3	0.15	0.50000	1.000
	13	1973.5	0.16234	0.5	0.3	0.15	0.50000	1.000
	14	1974.5	0.16262	0.5	0.3	0.15	0.50000	1.000
	15	1975.5	0.1629	0.5	0.3	0.15	0.50000	1.000
	16	1976.5	0.16317	0.5	0.3	0.15	0.50000	1.000
	17	1977.5	0.16345	0.5	0.3	0.15	0.50000	1.000
	18	1978.5	0.16372	0.5	0.3	0.15	0.50000	1.000
	19	1979.5	0.16399	0.5	0.3	0.15	0.50000	1.000
	20	1980.5	0.16426	0.5	0.3	0.15	0.50000	1.000
	21	1981.5	0.15976	0.38235	0.3	0.1	0.38235	1.000
	22	1982.5	0.15857	0.34775	0.3	0.1	0.34775	1.000
	23	1983.5	0.15841	0.33757	0.3	0.1	0.33757	1.000
	24	1984.5	0.15856	0.33458	0.3	0.1	0.33458	1.000

4. H^+ and AL^{3+} sorbed at the exchange complex (eq. 2) for Gaines Thomas

input file: vdp_6.in, output file vsdp_6.out

```
!VSDp base test file
!cH       : [H+] (eq/m3)
!cBc      : [Ca+Mg+K] (eq/m3)
!cCa      : [Ca] (eq/m3)
!cMg      : [Mg] (eq/m3)
!cK       : [K] (eq/m3)
!cNa      : [Na] (eq/m3)
!cAl      : [Al3+] (eq/m3)
!pH       : pH
!bsat     : EBc
!ECa      : ECa
!EMg      : EMg
!EK       : EK
!EH       : EH
!EAl      : EAl
```

	m	n	fac	Kvalue
lgKAlBc	6	3	2	0.888889	888888889
lgKHBc	5	1	2	2	200

```
KHBc = EfromLog(modExc,lgExcMat(1,3),1,2,3)  ! -> "eq/m3"
KAlBc = EfromLog(modExc,lgExcMat(2,3),3,2,3) ! -> "eq/m3"

   EfromLog  (modExc,lgK,m,n,lit)
x = m
y = n
   fac = n**x/m**y
         EfromLog = fac*10**(lgK+lit*(x-y))
```

!count	,time	,cH	,cBc	,cCa	,cMg	,cK	,cNa	,cAl	,pH	,bsat	,EH	,EAl	EH	check	EAl	check
0	1960.5	5.63E-03	1.5067	1.5	3.33E-03	3.33E-03	0.33333	5.36E-05	5.2494	0.57468	4.92E-02	0.37614	4.92E-02	1.000	0.3761	1.000
1	1961.5	5.10E-03	1.2516	1.2461	2.70E-03	2.70E-03	0.33333	3.99E-05	5.2922	0.57796	4.90E-02	0.373	4.90E-02	1.000	0.3730	1.000
2	1962.5	4.94E-03	1.1877	1.1827	2.51E-03	2.51E-03	0.33333	3.63E-05	5.3059	0.58109	4.89E-02	0.37	4.89E-02	1.000	0.3700	1.000
3	1963.5	4.89E-03	1.1749	1.1701	2.42E-03	2.42E-03	0.33333	3.51E-05	5.3105	0.58414	4.88E-02	0.36708	4.88E-02	1.000	0.3671	1.000
4	1964.5	4.87E-03	1.1749	1.1702	2.37E-03	2.37E-03	0.33333	3.46E-05	5.3128	0.58714	4.87E-02	0.36421	4.87E-02	1.000	0.3642	1.000
5	1965.5	4.85E-03	1.1782	1.1736	2.32E-03	2.32E-03	0.33333	3.42E-05	5.3144	0.59009	4.85E-02	0.36138	4.85E-02	1.000	0.3614	1.000
6	1966.5	4.83E-03	1.1824	1.1779	2.27E-03	2.27E-03	0.33333	3.39E-05	5.3158	0.59301	4.84E-02	0.35859	4.84E-02	1.000	0.3586	1.000
7	1967.5	4.82E-03	1.1869	1.1824	2.23E-03	2.23E-03	0.33333	3.36E-05	5.3171	0.59588	4.83E-02	0.35584	4.83E-02	1.000	0.3558	1.000
8	1968.5	4.80E-03	1.1914	1.1871	2.19E-03	2.19E-03	0.33333	3.32E-05	5.3184	0.59871	4.82E-02	0.35313	4.82E-02	1.000	0.3531	1.000
9	1969.5	4.79E-03	1.1961	1.1918	2.15E-03	2.15E-03	0.33333	3.30E-05	5.3197	0.6015	4.80E-02	0.35046	4.80E-02	1.000	0.3505	1.000
10	1970.5	4.78E-03	1.2007	1.1965	2.11E-03	2.11E-03	0.33333	3.27E-05	5.3209	0.60425	4.79E-02	0.34784	4.79E-02	1.000	0.3479	1.000

The Gaines-Thomas equation for exchange reads:

$$\frac{E_{Al}^2}{E_{Bc}^3} = k_{AlBc}\frac{[Al]^2}{[Bc]^3} \quad \text{and} \quad \frac{E_H^2}{E_{Bc}} = k_{HBc}\frac{[H]^2}{[Bc]}$$

5. H^+ and AL^{3+} sorbed at the exchange complex (eq. 2) for Gapon

```
input file: vdp_7.in, output file vsdp_7.out
!cBc      : [Ca+Mg+K] (eq/m3)
!cNa      : [Na] (eq/m3)
!cCl      : [Cl] (eq/m3)
!cAl      : [Al3+] (eq/m3)
!cH       : [H+] (eq/m3)
!bsat     : EBc
!EH       : EH
!EAl      : EAl
!pH       : pH
```

	m	n	x	y	fac	Kvalue
lgKAlBc	1	3	2	0.5	0.333333	0.980561	31.00806
lgKHBc	0	1	2	0.5	1	1.414214	0.044721

```
KHBc = EfromLog(modExc,lgExcMat(1,3),1,2,3)  ! -> "eq/m3"
KAlBc = EfromLog(modExc,lgExcMat(2,3),3,2,3) ! -> "eq/m3"

EfromLog  (modExc,lgK,m,n,lit)
    x = 1./n
    y = 1./m
  fac = n**x/m**y
  EfromLog = fac*10**(lgK+lit*(x-y))
```

!count	,time	,cBc	,cNa	,cCl	,cAl	,cH	,bsat	,EH	,EAl	,pH	EH	check	EAl	check
0	1960.5	1.5067	0.33333	0.33333	5.36E-05	5.63E-03	0.51219	1.05E-04	0.48771	5.2494	1.05E-04	1.000	0.4877	1.000
1	1961.5	1.252	0.33333	0.33333	3.90E-05	5.07E-03	0.51545	1.04E-04	0.48444	5.2953	1.04E-04	1.000	0.4844	1.000
2	1962.5	1.1881	0.33333	0.33333	3.47E-05	4.87E-03	0.51858	1.04E-04	0.48132	5.3121	1.04E-04	1.000	0.4813	1.000
3	1963.5	1.1752	0.33333	0.33333	3.29E-05	4.79E-03	0.52163	1.03E-04	0.47827	5.3198	1.03E-04	1.000	0.4783	1.000
4	1964.5	1.1751	0.33333	0.33333	3.18E-05	4.73E-03	0.52463	1.02E-04	0.47527	5.3251	1.02E-04	1.000	0.4753	1.000
5	1965.5	1.1783	0.33333	0.33333	3.08E-05	4.68E-03	0.52758	1.02E-04	0.47231	5.3296	1.02E-04	1.000	0.4723	1.000
6	1966.5	1.1823	0.33333	0.33333	2.99E-05	4.63E-03	0.5305	1.01E-04	0.4694	5.334	1.01E-04	1.000	0.4694	1.000
7	1967.5	1.1866	0.33333	0.33333	2.90E-05	4.59E-03	0.53338	1.01E-04	0.46652	5.3382	1.01E-04	1.000	0.4665	1.000
8	1968.5	1.1911	0.33333	0.33333	2.82E-05	4.55E-03	0.53621	9.99E-05	0.46369	5.3423	9.99E-05	1.000	0.4637	1.000
9	1969.5	1.1956	0.33333	0.33333	2.74E-05	4.50E-03	0.539	9.93E-05	0.4609	5.3464	9.93E-05	1.000	0.4609	1.000
10	1970.5	1.2001	0.33333	0.33333	2.67E-05	4.46E-03	0.54175	9.87E-05	0.45815	5.3504	9.87E-05	1.000	0.4582	1.000

The exchange equation for Gapon reads:

$$\frac{E_{Al}}{E_{Bc}} = k_{AlBc}\frac{[Al]^{1/3}}{[Bc]^{1/2}} \quad \text{and} \quad \frac{E_{H}}{E_{Bc}} = k_{HBc}\frac{[H]}{[Bc]^{1/2}}$$

6. Computation of the carbon pool (eq. 4,5,8,16,17,19)

```
input file: vdp_3.in, output file vsdp_3.out
!Clf      : C litterfall (g C/m2/yr)
!Cpool    : Total C pool (g C/m2)
!DPM      : Decomposable litter (g/m2)
!RPM      : Recalcitrant litter (g/m2)
!BIO      : Microbial biomass (g/m2)
!HUM      : Humified matter (g/m2)
!IOM      : Inert organic matter (g/m2)
!Nmi      : N mineralised (eq/m2/yr)
!CNrat    : Average soil C:N (g/g)
```

rfmi	1
ctclay	5
Qlf	0.25

par(1) = 10. *rfmi * 0.6 ! kDPM	6.00
par(2) = 0.3 *rfmi * 0.6 ! kRPM	0.18
par(3) = 0.66*rfmi * 0.6 ! kBIO	0.40
par(4) = 0.02*rfmi * 0.6 ! kHUM	0.01
h1 = 1.67 * (1.85 + 1.60*exp(-0.0786* ctclay))	4.89
par(6) = 1/(h1+1) ! 1-frCO2	0.17
par(7) = 0.46 ! frBIO	0.46
par(8) = 1 ! N -> BIO+HUM	1.00

!count	,time	,Clf	,Cpool	,DPM	,RPM	,BIO	,HUM	,IOM	HUM eq 19	checkHUM	DPMin (eq 8)	RPMin (eq 8)	DPM0 (eq 16)	kDPM	DPM(t) (eq 4)	RPM0 (eq 17)	kRPM	RPM(t) (eq 5)	checkDPM	checkRPM
0	1960.5	400	4980.6	80.232	2072.2	95.563	2310.6	422.01	2310.6	1.000	80	320	93.33	0.2314	80.23	2097.78	1752.21	2072.21	1.000	1.000
1	1961.5	400	4975.4	80.2	2050.9	94.969	2327.4	422.01	2327.3	1.000	80	320	80.23	0.1989	80.20	2072.21	1730.86	2050.86	1.000	1.000
2	1962.5	400	4973.3	80.2	2033	94.339	2343.7	422.01	2343.8	1.000	80	320	80.20	0.1988	80.20	2050.86	1713.02	2033.02	1.000	1.000
3	1963.5	400	4973.6	80.2	2018.1	93.723	2359.6	422.01	2359.6	1.000	80	320	80.20	0.1988	80.20	2033.02	1698.12	2018.12	1.000	1.000
4	1964.5	400	4976	80.2	2005.7	93.148	2375	422.01	2374.9	1.000	80	320	80.20	0.1988	80.20	2018.12	1685.68	2005.68	1.000	1.000
5	1965.5	400	4980.2	80.2	1995.3	92.628	2390.1	422.01	2390.1	1.000	80	320	80.20	0.1988	80.20	2005.68	1675.28	1995.28	1.000	1.000
6	1966.5	400	4985.8	80.2	1986.6	92.167	2404.8	422.01	2404.8	1.000	80	320	80.20	0.1988	80.20	1995.28	1666.60	1986.60	1.000	1.000
7	1967.5	400	4992.5	80.2	1979.3	91.766	2419.2	422.01	2419.2	1.000	80	320	80.20	0.1988	80.20	1986.60	1659.35	1979.35	1.000	1.000
8	1968.5	400	5000.3	80.2	1973.3	91.421	2433.3	422.01	2433.4	1.000	80	320	80.20	0.1988	80.20	1979.35	1653.29	1973.29	1.000	1.000
9	1969.5	400	5008.8	80.2	1968.2	91.127	2447.2	422.01	2447.3	1.000	80	320	80.20	0.1988	80.20	1973.29	1648.23	1968.23	1.000	1.000
10	1970.5	400	5018	80.2	1964	90.88	2460.9	422.01	2460.9	1.000	80	320	80.20	0.1988	80.20	1968.23	1644.00	1964.00	1.000	1.000

7. Carbon in the IOM pool (eq. 15)

```
input file: vdp_3.in, output file vsdp_3.out
!Clf      : C litterfall (g C/m2/yr)
!Cpool    : Total C pool (g C/m2)
!DPM      : Decomposable litter (g/m2)
!RPM      : Recalcitrant litter (g/m2)
!BIO      : Microbial biomass (g/m2)
!HUM      : Humified matter (g/m2)
!IOM      : Inert organic matter (g/m2)
!Nmi      : N mineralised (eq/m2/yr)
!CNrat    : Average soil C:N (g/g)
```

rfmi	1
ctclay	5
Qlf	0.25
Cpool_0	5000

Falloon:

!count	,time	,Clf	,Cpool	,DPM	,RPM	,BIO	,HUM	,IOM
0	1960.5	400	4980.6	80.232	2072.2	95.563	2310.6	422.01

the mean. Hence a model for IOM based upon total SOC (both in t C ha^{-1}) was constructed (Fig. 1), using log functions, which accounted for 63.4% of the variance in IOM ($t_{26} = 6.91$, $P < 0.001$). The model equation is given below:

$$\log \mathrm{IOM} = -1.31\ (\mathrm{S.E.}\ 0.28) + 1.139\ (\mathrm{S.E.}\ 0.165) \times \log \mathrm{SOC} \quad (1)$$

which is equivalent to

$$\mathrm{IOM} = 0.049 \times \mathrm{SOC}^{1.139} \quad (2)$$

IOM eq 15	IOM source code	Falloon (in ton/ha)
223.9237626	422.0102	4.201

8. N mineralisation (eq. 11) and C/N ratio in the DPM pool (eq. 12)

```
input file: vdp_4.in, output file vsdp_4.out
!Cpool    : Total C pool (g C/m2)
!Npool    : Total N pool (g/m2)
!CNrat    : Average soil C:N (g/g)
!Nlf      : N litterfall (g N/m2/yr)
!Nmi      : N mineralised (eq/m2/yr)
!DPM      : Decomposable litter (g/m2)
```

rfmi	1
ctclay	5
Qlf	0.25
Clf	400

DPMin	80
RPMin	320

!count	,time	,Cpool	,Npool	,CNrat	,Nlf	,Nmi	,DPM	,RPM
0	1960.5	4980.6	130.92	38.044	10	0.2916	80.232	2072.2
1	1961.5	4975.4	137.24	36.253	10	0.26245	80.2	2050.9
2	1962.5	4973.3	143.54	34.648	10	0.26458	80.2	2033
3	1963.5	4973.6	149.8	33.201	10	0.26675	80.2	2018.1
4	1964.5	4976	156.04	31.889	10	0.26889	80.2	2005.7
5	1965.5	4980.2	162.25	30.695	10	0.27102	80.2	1995.3
6	1966.5	4985.8	168.42	29.603	10	0.27317	80.2	1986.6
7	1967.5	4992.5	174.57	28.6	10	0.27533	80.2	1979.3
8	1968.5	5000.3	180.68	27.674	10	0.2775	80.2	1973.3
9	1969.5	5008.8	186.77	26.819	10	0.27969	80.2	1968.2
10	1970.5	5018	192.82	26.024	10	0.28188	80.2	1964
11	1971.5	5027.7	198.84	25.285	10	0.28409	80.2	1960.5
12	1972.5	5037.8	204.83	24.594	10	0.28631	80.2	1957.5
13	1973.5	5048.2	210.79	23.948	10	0.28853	80.2	1955.1
14	1974.5	5058.9	216.72	23.342	10	0.29076	80.2	1953
15	1975.5	5069.7	222.62	22.773	10	0.29299	80.2	1951.3
16	1976.5	5080.7	228.49	22.236	10	0.29521	80.2	1949.9
17	1977.5	5091.8	234.33	21.73	10	0.29743	80.2	1948.7
18	1978.5	5103	240.13	21.251	10	0.29965	80.2	1947.7
19	1979.5	5114.1	245.9	20.797	10	0.30186	80.2	1946.8
20	1980.5	5125.3	251.65	20.367	10	0.30408	80.2	1946.1
21	1981.5	5136.5	257.36	19.958	10	0.30628	80.2	1945.5
22	1982.5	5147.6	263.04	19.57	10	0.30847	80.2	1945

CNdpm eq12	check
11.7647318	1.00

Computation Nmi (eq 11)
Timestep 1 (results from debugging model):

CPOOL(1)	0.199823		cn(1)	11.76471	0.001213
CPOOL(2)	1730.856		cn(2)	100	1.236326
CPOOL(3)	94.96871		cn(3)	15	0.452232
CPOOL(4)	2327.399		cn(4)	37.91452	4.384673
CPOOL(5)	422.0102		cn(5)	10	3.014359
sum	4575.434	4975.434			9.088803
COLD(1)	80.23245		cnOLD(1)	11.76471	0.487125
COLD(2)	2072.211		cnOLD(2)	100	1.480151
COLD(3)	95.56254		cnOLD(3)	15	0.45506
COLD(4)	2310.553		cnOLD(4)	42.16043	3.914559
COLD(5)	422.0102		cnOLD(5)	10	3.014359
sum	4980.569				9.351254
				Nmi eq 11:	0.262451
				check	1.000

9. N nitrification (eq. 21) and denitrification (eq. 22)

input file: vdp_5.in, output file vsdp_5.out

```
!NOxdep  : NOx deposition (eq/m2/yr)
!NH3dep  : NH3 deposition (eq/m2/yr)
!cNO3    : [NO3-] (eq/m3)
!cNH4    : [NH4+] (eq/m3)
!Nupt    : N storage+litterfall (eq/m2/yr)
!pH      : pH
!Nmi     : N mineralised (eq/m2/yr)
!Nni     : N nitrified (eq/m2/yr)
!Nde     : N denitrified (eq/m2/yr)
```

thick	0.5
theta	0.25
Kni_ref	4
rf_ni	1
fn2o_ni	0
Kde_ref	4
rf_denit	0.1

!count	,time	,NOxdep	,NH3dep	,cNO3	,cNH4	,Nupt	,pH	,Nmi	,Nni	,Nde	NO3in	NH4in	kniph (eq 22)	fni	Nni	check	kdeph (eq 23)	fde	Nde	check
0	1960.5	5.00E-02	4.00E-02	1.13E+00	1.92E-02	2.50E-02	3.7731	2.92E-01	0.30084	1.05E-02	4.93E-01	3.09E-01	3.9343	0.98044	3.03E-01	1.007	0.0178	0.0176	8.69E-03	0.828
1	1961.5	5.00E-02	4.00E-02	1.08E+00	1.29E-02	2.50E-02	3.778	2.62E-01	0.27438	8.22E-03	4.59E-01	2.79E-01	3.9356	0.98047	2.74E-01	0.997	0.0180	0.0178	8.19E-03	0.996
2	1962.5	5.00E-02	4.00E-02	1.06E+00	1.29E-02	2.50E-02	3.7793	2.65E-01	0.2757	8.21E-03	4.59E-01	2.81E-01	3.9359	0.98047	2.76E-01	1.000	0.0181	0.0179	8.21E-03	0.999
3	1963.5	5.00E-02	4.00E-02	1.06E+00	1.30E-02	2.50E-02	3.7792	2.67E-01	0.27783	8.25E-03	4.61E-01	2.83E-01	3.9359	0.98047	2.78E-01	1.000	0.0181	0.0179	8.25E-03	1.000
4	1964.5	5.00E-02	4.00E-02	1.07E+00	1.31E-02	2.50E-02	3.7786	2.69E-01	0.27994	8.28E-03	4.64E-01	2.86E-01	3.9357	0.98047	2.80E-01	1.000	0.0180	0.0179	8.28E-03	1.000
5	1965.5	5.00E-02	4.00E-02	1.08E+00	1.32E-02	2.50E-02	3.778	2.71E-01	0.28205	8.32E-03	4.67E-01	2.88E-01	3.9356	0.98047	2.82E-01	1.000	0.0180	0.0178	8.32E-03	1.000
6	1966.5	5.00E-02	4.00E-02	1.08E+00	1.33E-02	2.50E-02	3.7773	2.73E-01	0.28416	8.36E-03	4.70E-01	2.90E-01	3.9354	0.98046	2.84E-01	1.000	0.0180	0.0178	8.36E-03	1.000
7	1967.5	5.00E-02	4.00E-02	1.09E+00	1.34E-02	2.50E-02	3.7766	2.75E-01	0.28629	8.40E-03	4.73E-01	2.92E-01	3.9352	0.98046	2.86E-01	1.000	0.0179	0.0178	8.40E-03	1.000
8	1968.5	5.00E-02	4.00E-02	1.10E+00	1.35E-02	2.50E-02	3.7759	2.78E-01	0.28843	8.44E-03	4.76E-01	2.94E-01	3.9350	0.98046	2.88E-01	1.000	0.0179	0.0178	8.44E-03	1.000
9	1969.5	5.00E-02	4.00E-02	1.10E+00	1.36E-02	2.50E-02	3.7751	2.80E-01	0.29058	8.48E-03	4.79E-01	2.96E-01	3.9348	0.98045	2.91E-01	1.000	0.0179	0.0177	8.48E-03	1.000
10	1970.5	5.00E-02	4.00E-02	1.11E+00	1.37E-02	2.50E-02	3.7744	2.82E-01	0.29275	8.52E-03	4.82E-01	2.99E-01	3.9346	0.98045	2.93E-01	1.000	0.0178	0.0177	8.52E-03	1.000

Annex 4 Code check of CNRothC.f90

Steady States of C-pools in VSD+

Max.Posch@RIVM.NL, 18 Oct 2016

In the following the steady state equations for the C-pools BIO and HUM are derived and compared with equations in the VSD+ paper (Bonten *et al.,* 2016; 'the paper' in the following) and the code in the Fortran subroutines:

We have:

(A) $k_{DPM}DPM + k_{RPM}RPM = C_{lf}$

We define for convenience:

(B) $x = k_{BIO}BIO$ and $y = k_{HUM}HUM$

Furthermore we define (see eq.9 in the paper):

(C) $h_1 = CO_2/(BIO + HUM)$

And thus obtain (see eq.10; *f* instead of *fr*):

(D) $f_{CO2} = \frac{h_1}{1+h_1} \quad \Rightarrow \quad h_1 = \frac{f_{CO2}}{1-f_{CO2}}$

Then the steady-state equations *BIO* (x) and *HUM* (y) read according to eqs.6 and 7 in the paper ($d./dt$=0):

(E) $0 = -x + (1 - f_{CO2})f_{BIO}(C_{lf} + x + y)$

and

(F) $0 = -y + (1 - f_{CO2})(1 - f_{BIO})(C_{lf} + x + y)$

Adding the two equations yields:

(G) $x + y = (1 - f_{CO2})(C_{lf} + x + y)$

And from this we get (using eq.D):

(H) $x + y = \frac{1}{h_1}C_{lf}$

Inserting this into eqs.E and F yields, resp (see eq.B):

(I) $BIO = \frac{f_{BIO}C_{lf}}{k_{BIO}}\left(\frac{1}{f_{CO2}} - 1\right) = \frac{f_{BIO}C_{lf}}{k_{BIO}h_1}$

and

(J) $HUM = \frac{(1-f_{BIO})C_{lf}}{k_{HUM}}\left(\frac{1}{f_{CO2}} - 1\right)$

Eq.J is not given in the paper, whereas eq.I is identical to eq.18 in the paper, if one drops the extra factor f_{BIO} (as agreed); and eq.I is also equal to Cpool(3) as coded in the subroutine 'CNRothCstst'.

Discussion

What triggered my/our 'interest' in the first place was that for f_{CO2}=0, BIO (and HUM) becomes infinite! In practice, this is never the case, as h_1 (and thus f_{CO2}) is always > 0 (see eq.9 in the paper). This 'interesting' behaviour follows (of course) from the mass balance equations: From f_{CO2}=0 follows h_1=0, and eq.G then reads:

(G') $x + y = C_{lf} + x + y$

which, for C_{lf} > 0, can never be fulfilled, except for $x+y=\infty$ … an interesting model feature!

Annex 5 Uncertainty of critical loads

The critical loads, used in the Dutch policy, are based on calculations with SMART2 by Van Dobben *et al.* (2006) and they performed a sensitivity and uncertainty analyses. One of the difficulties in that study was to get a relation between Ellenberg-N (an indicator for nutrient richness of a habitat which can be derived from species composition) and a related model output. This was needed to get a boundary condition for the calculation of the critical load. Therefore, historical runs were made with SMART2 with modelled N-availability for the years of the observed species composition. A regression between Ellenberg-N and the calculated N availability by SMART2 was used get N-availability as a boundary condition for critical loads. The unexplained system variation of the regression between Ellenberg-N and N availability had a large contribution to the uncertainty of critical loads for nitrogen.

In 2014, we tried to reduce the uncertainty in critical loads by leaving out the conversion between Ellenberg-N and N availability and replace the boundary condition by measured NO3 contents in the soil ($mg.kg^{-1}$). As mentioned in section 6.2.2 the results were too uncertain to publish these critical loads for the Dutch policy. Here, we show just a short qualitative analyses of that uncertainty.

With the method, new uncertainties were introduced. Again a conversion was needed to link a boundary condition to model output, in this case the conversion from NO_3 content in the soil to NO_3 concentration is soil solution. One needs the bulk density of the soil and the volumetric moisture content of the soil to make the conversion. Bulk density was in the database of the measured NO_3 contents, so we had to estimate it for different soil types. This resulted in a uncertainty in the boundary condition itself.

We did several calculations with different calculations of soil moisture reduction functions. One with the reduction functions for soil moisture with soil moisture from the database, one with soil moisture contents derived from Mean Spring water table (MSW) in the database, and one with the reduction functions from SMART2, which are directly related to MSW. The results are compared in Figure A5.1. The differences between the calculations with different reduction functions seems higher when pH is taken as boundary condition. Further research is needed to link model output to nutrient richness.

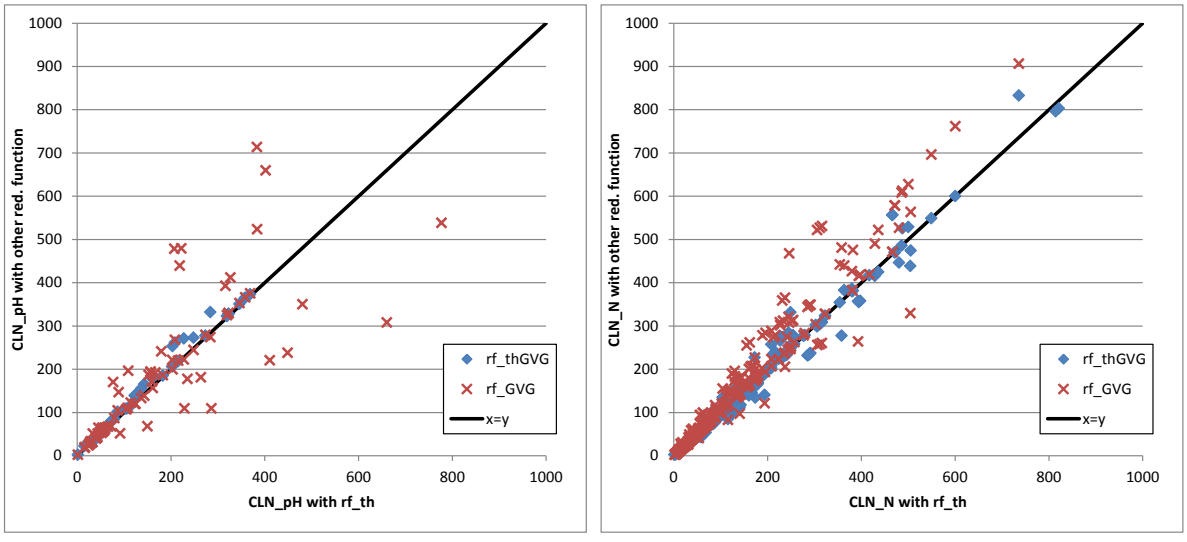


Figure A5.1 *Critical loads for nitrogen calculated with reduction function with soil moisture from the database compared with calculations with reduction functions based on soil moisture derived from MSW and reduction function based on MSW. Left figure shows the results for pH as boundary condition and right NO_3 concentration as boundary condition.*

Annex 6 Issues from workshops

April 2012

MetHyd:

- Allow for sunshine input in W/m^2 instead of % [Max/GJ]
- PAR: no units; how to get from RAD: auto convert from watts to mmol/s (Luc: mmol fotons?)
- Entry for PAR in Help-file [Max/GJ]
- Allow choice of PTF for bulk density calculation (already in Fortran code) [GJ/Max]
- Describe layout of ascii file with meteo data [GJ/Max]

GrowUp:

- correct versioning (v. 1.1?) [GJ/Luc]
- 'share' of what? (cover, volume, mass …) [Luc] → discus with Martjan
- default directory stored in registry to avoid AppData use all of the time [GJ]
- What is the use of the 'delete last row' button in Stem Growth and Management table? [GJ]
- What does 'Read N deposition' button do? [GJ]
- Is default management country/regio specific? [GJ] → include in help, only per species
- Countries are not completely in alphabetical order Also 'Serbia and Montenegro' and 'Montenegro'. [GJ]
- Can tree species be organised hierarchically, e.g.: [GJ]

  Mixed
  Broadleaves
  — Hard broadleaves
  — Carpinus
  — Quercus
  — Quercus faginea
  …
  Coniferous
- Inconsistencies in tree species list: [GJ]
  - Names are in latin and english (should be either one of these)
  - Some name are twice in (e.g. oak and quercus, larch and larix)
- Stem growth in growup and growup help is in m3/yr. Shouldn't this be m3/ha/yr? [GJ]
- In the tab results litterfall and soil inputs should be in g/m2/yr (now: g/m2) and uptake in eq/m2/yr (now: eq/m2) [GJ]
- Management table does not completely fit. [GJ] → drop down menu
- Total share of cohorts is now scaled to 100%. This goes wrong when a new cohort is introduced while an old cohort is still standing. → no scaling and introduce cover graph; give warning is cover exceeds 100% at any moment [GJ]
- averaging of : is now only shown for simulation period and not outside. When no scaling 'average' should be 'sum'(?) [GJ]
- BC uptake can be negative even for no management. Reason: inconsistency between growth and BEFs [Luc/Martjan]
- there should be an error message when no time period is available in vsdp input file in growup, now growup crashes [GJ]
- Include natural rejuvenation in management [Luc/GJ]
- BEFs seem too high for a number of countries, review of BEFs [Luc/Martjan]
- output of Growup is one year wrong, e.g. output for 1960 as given by growup should be 1959 (version 1.2) [GJ]

VSD+:

- Other nature types than forests (?) <Luc: technically there is no restrictions on applying VSD+ to other vegetation types than forest, question is to which extent default CNorg parameters are correct then? Review of CNorg with WU soil biologist is foreseen> [Luc]
- calibration of C pool for other nature types: contact Julian Aherne [Luc]
- calibration of CN org defaults on AU and CH data [Luc/Dani/Thomas D.]
- new file run: cannot open data file for write; save close app open : OK (must be missing path to AppData) [GJ]
- Default values given by the interface are different from the ones in the help file for the individual parameters [Luc/GJ]
- stand-alone dll with calling convention (see e.g. c_vsd.c), at least distribute to DK and DE [GJ/Luc] → done for DK
- cmin is called but no longer used [Luc/GJ]

Access (Jaap):

- if G3 is chosen all sub-coded plants should be included as well
- in texts: 'fraction' → 'share'; 'Pare' → 'PAR'

April 2013

Comments and ideas from VSD+ training session, Copenhagen 2013

VSD+ Studio

- how to calculate effects on non-forest vegetations; include other vegetation models (BERN, PROPS, MOVE) (to be discussed)
- select species by choosing EUNIS class in VSD+ studio (Gert Jan)
- tabs in observation data file gives error in studio; must be in the fortran/C++ check of the observations (Gert Jan)
- reformat VEG output (how?) (Gert Jan)
- add table to VSDp help file to indicate which data are needed to calibrate certain parameters (Gert Jan)
- calcareous soils in VSD+?, e.g. Italy has many calcareous soils (if yes: Luc, Max)
- parameters that should be calibrated can now typed directly, prevent this (Gert Jan)
- remove Nimm_acc from Help text (VSD+ Studio > Bayesian Calibration) (Gert Jan)

GrowUp

- standing biomass and litterfall output to single file for all organs (Gert Jan)
- graph of stem biomass as m3/ha (Gert Jan)
- update chemical composition of litterfall by using data from level II plots (at least Austria has these data) and Fundiv data (Luc) → requires recalibration of CNorg parameters
- take ctrl-o out of help file for 'open file' (Gert Jan)
- make turnover rates for evergreen foliage region dependent (they can be as low as 0.07 yr-1 in Northern regions, pers. comm. Dani) (Luc, Gert Jan)
- correct interpolation of BEFs (Luc)
- evaluate BEF using data from Austria and chronosequences (Luc)
- when opening an 'old' growup file forest type is set to natural rejuvenation. Uniform age should be default (Gert Jan)

MetHyd

- output of multiple (non-VSD+) variables in single file (Gert Jan)

October 2013

GrowUp:

- Update help file GrowUp

MetHyd:

- Change to meters for ps and percol

VSD+

- Average species occurrence next to occurrence for species and groups
- Precip input as result from MetHyd
- Mouse over line show species
- Output of vegetation model: option for all species or selected
- Isoline add-on
- Cutoff implementation
- Correct file with EVM-EUNIS for forests
- Sort EVM alphabetically per EUNIS class
- EVM-EUNIS for EUNIS level 2
- C/N pool modelling
- Database name PROPS written to output file from props
- No spaces in names in PROPS output

General:

- Make new installs for MetHyd, GrowUp and VSD+PROPS
- DLL's to Jaap at CCE

PROPS:

- New data for PROPS: Austrian data, Irish data (received already), Finnish
- Derivation of new response functions
- Multiple models (different sets of abiotic factors)

Annex 7 Checklist Quality level A (in Dutch)

Status A voor simulatiemodellen

Continu verbeteren en productkwaliteit
Het op een niveau brengen en houden van de kwaliteit van operationele modellen is een continu proces. Verbeteracties worden regelmatig gepland en geëvalueerd in samenhang met toepassingen van het model. Voor de productkwaliteit zijn objectieve, verifieerbare criteria ontwikkeld.

Kwaliteitscriteria
We hebben twee kwaliteitsniveaus ingesteld met bijbehorende criteria:
- Status A. Het minimum kwaliteitsniveau waaraan alle operationele modellen moeten voldoen (deze checklist).
- Status AA. Het goede kwaliteitsniveau.

Bijna alle criteria voor kwaliteitsniveau Status A zijn statisch, dat wil zeggen dat aan alle van toepassing zijnde criteria moet worden voldaan om dit minimum kwaliteitsniveau te halen. De criteria voor Status AA zijn deels statisch en deels dynamisch. Dynamische criteria wil zeggen dat er planmatig aan gewerkt wordt om aan deze criteria te voldoen, bijvoorbeeld aan het verder valideren van het model.

Toekennen status en beroep
Om een kwaliteitsstatus te verkrijgen, moet een audit worden gehouden door een gekwalificeerde auditor of auditteam. Van de audit wordt door de auditor(s) een verslag gemaakt. Gewoonlijk zal de ingevulde checklist, met verwijzingen naar de relevante documentatie, voldoen als verslag. De auditee moet de verslaglegging goedkeuren. Bij verschil van mening beslist de softwarekwaliteitsmanager, indien hij geen deel uitmaakt van het auditteam. De directie beslist uiteindelijk als het verschil van mening blijft bestaan. Voor Status A moet voldaan worden aan de van toepassing zijnde Status A kwaliteitscriteria. Voor Status AA moet voldaan worden aan de van toepassing zijnde Status A én Status AA kwaliteitscriteria. De status wordt toegekend door de softwarekwaliteitsmanager.

Kwaliteitsdocumentatie
De beoordeling wordt gedaan aan de hand van schriftelijke documentatie, de 'kwaliteitsdocumentatie' van het model. Voor de indeling van de kwaliteitsdocumentatie kan de indeling van de checklist worden aangehouden. In ieder geval dient de documentatie van theorie, de technische- en gebruikersdocumentatie publiekelijk toegankelijk te zijn (bijvoorbeeld internet, WEnR(Alterra)-rapporten, publicaties).

Verantwoordelijkheden
De beheerders van het bestand zijn verantwoordelijk voor de kwaliteit van het model en voor het bijhouden van de kwaliteitsdocumentatie. De projectleider van het project dat het model toepast, is verantwoordelijk voor de kwaliteit van die toepassing.

Invullen checklist
De checklist wordt grotendeels door de auditee ingevuld: Algemeen, de 'kwaliteitsdocumentatie' waarnaar verwezen wordt (Verwijzingen) en bij elke vraag de verwijzing naar de relevante passage van de documentatie. De auditee kan ook opmerkingen en aanvullingen bij de vragen maken. Tijdens de audit vult de auditor zijn bevindingen in.

Meer informatie
De site Kwaliteit modellen en bestanden geeft meer informatie over het kwaliteitssysteem voor modellen en bestanden. Ook zijn daar voorbeelden, templates en 'handreikingen' te vinden.
Zijn er nog steeds vragen of onduidelijkheden? Of heb je behoefte aan ondersteuning? Neem dan contact op met de softwarekwaliteitsmanager.

Wijzigingen ten opzichte van vorige versies

Versie 1.0 (gepubliceerd)
21-9-2004, Jûnt Halbertsma
1. Eerste publicatie na discussie met onderzoekers.

Versie 1.1 (gepubliceerd)
9-3-2006, Jûnt Halbertsma
1. Tabel "Verwijzingen" toegevoegd.
2. Velden "opmerking" bij de vragen uitgesplitst voor auditor en auditee.
3. Velden "verwijzing" bij de vragen toegevoegd.
4. Tekst van inleiding aangepast op de wijzigingen.

Versie 2.0 (gepubliceerd)
27-12-2007, Jûnt Halbertsma
1. Toelichting uitgebreid en direct bij vragen gezet.
2. Header aangepast.
3. Checklists Status A en Status AA gesplitst.
4. Slecht werkende formulier functionaliteit van Word verwijderd.

Algemeen	
Naam model/bestand	VSD+
Versienummer	1.4
Versiedatum	16-06-2015
Korte omschrijving	VSD^+ beschrijft de bodemchemie, koolstofvastlegging en nutriëntenkringloop in natuurlijke systemen
Doelgebied	Natuurlijke terrestrische ecosystemen, puntschaal tot Europees (losse gridcellen)
Database omgeving	nvt
Programmeertaal	Fortran90 (rekenkern), C++ (schil)
Platform	Windows XP and higher
Beheerder/ contactperso(o)n(en)	Janet Mol / Gert Jan Reinds

Verwijzingen	
I.	VSD: Posch and Reinds (2009): http://www.sciencedirect.com/science/article/pii/S1364815208001734
II.	Bonten, L.T.C., G.J. Reinds and M. Posch. 2016. A model to calculate effects of atmospheric deposition on soil acidification, eutrophication and carbon sequestration. Environmental Modelling & Software 79 (2016) 75-84
III.	Mol-Dijkstra, J.P. and G.J. Reinds (2017). Technical documentation of the VSD+ model. Status A. WOt-technical report 88. WOT Natuur & Milieu, WUR, Wageningen
IV.	Bonten L, Posch M, Reinds GJ, 2010. The VSD+ Soil Acidification Model – Model Description and User Manual. Alterra and CCE, Wageningen and Bilthoven. (VSD_help.chm)
V.	Beheer & Jaarplan 2017

Checklist Status A simulatiemodellen

Beoordeling
Voor het verkrijgen van Status A moet een audit worden gehouden door een gekwalificeerde auditor of auditteam. Van de audit wordt door de auditor(s) een verslag gemaakt. Gewoonlijk zal de ingevulde checklist, met verwijzingen naar de relevante documentatie, voldoen als verslag. De auditee moet de verslaglegging goedkeuren. Status A wordt gehaald als aan alle van toepassing zijnde criteria wordt voldaan. De status wordt verleend door de softwarekwaliteitsmanager.
De beoordeling wordt gedaan aan de hand van schriftelijke documentatie, de "kwaliteitsdocumentatie" van het model. De documentatie van theorie, de technische- en gebruikersdocumentatie dient publiekelijk toegankelijk te zijn (b.v. internet, Alterra rapporten, publicaties).

Status A toegekend:		datum:	beoordeeld door:	
			naam:	handtekening:
☑ ja	☐ nee	08 feb 2017	George van Voorn Geerten Hengeveld Janien van der Greft	

Theorie
In dit deel wordt de wetenschappelijke achtergrond van het model beschreven. Beschrijf het conceptuele en mathematische model en de overwegingen en aannamen die hieraan ten grondslag liggen. Een publicatie is een publiek toegankelijk document, waaronder dus ook een web-site en een Alterra rapport valt. Het verdient de voorkeur deze documentatie in het engels te schrijven.
Kijk op de site "Kwaliteit modellen en bestanden" voor voorbeelden, templates en "handreikingen".

		ja	nee	n.v.t.
A 1	Is de theoretische onderbouwing van het model omschreven?	☑	☐	☐
	verwijzing: VSD: I/ 1 & 2 VSD+: II/ 1 & 2.1			
	opmerking auditee:			
	opmerking auditor:			
	Toelichting: Beschrijf het conceptuele model met de overwegingen die hieraan ten grondslag liggen. Motiveer de gekozen aannamen en vereenvoudigingen (vraag A4). Beschrijf het mathematische model.			
A 2	Is het doel waarvoor het model is ontworpen beschreven?	☑	☐	☐
	verwijzing: III/ 1 & 2.1			
	opmerking auditee:			
	opmerking auditor:			
	Toelichting: Licht toe waarom het model is gemaakt.			
A 3	Is het toepassingsgebied van het model beschreven?	☑	☐	☐
	verwijzing: III/ 2.1			
	opmerking auditee:			
	opmerking auditor:			
	Toelichting: Beschrijf in welke situaties het model wel en niet kan worden toegepast. Denk hier ook aan het spatiele en temporele schaalniveau.			

A 4	Zijn de vereenvoudigingen en aannamen over de gebruikte representatie van de werkelijkheid gemotiveerd en beschreven? verwijzing: III/ 2.2 opmerking auditee: Initialisatie vanuit invoer wordt niet ondersteund opmerking auditor: Toelichting: Beschrijf en motiveer de aannamen om tot het conceptuele model te komen.	☑	☐	☐

Technische documentatie

In dit deel wordt de vertaling van het mathematisch model naar de computercode beschreven voor ontwikkelaars. Het computerprogramma wordt gedocumenteerd op een manier dat een opvolger voldoende informatie heeft om het programma te onderhouden en verder te ontwikkelen.
Het verdient de voorkeur deze documentatie in het engels te schrijven.
Kijk op de site "Kwaliteit modellen en bestanden" voor voorbeelden, templates en "handreikingen".

		ja	nee	n.v.t.
A 5	Is er een document met metainformatie van het model? verwijzing: III/ 3.1 opmerking auditee: opmerking auditor: Toelichting: Onder metainformatie van het model wordt verstaan die informatie die een gebruiker nodig heeft om te kunnen beslissen of hij dit model voor zijn probleem kan gebruiken. Denk hierbij o.a. aan: – Naam, versie en releasedatum van het model – Wat doet het? – Wat is het toepassingsgebied? – Wat is het schaalniveau (temporeel en spatieel)? – Welke invoer is nodig? – Welke uitvoer produceert het? – Hoe communiceert het model met de gebruiker en in welke taal? – Op welk platform (Windows, Linux, e.d.) draait het? – Wordt het model uitgeleverd? – Wat kost het? – Wie is de contactpersoon? De metainformatie staat bij voorkeur voorin de technische documentatie en de gebruikersdocumentatie of op (of vlakbij) de startpagina van de web site van het model.	☑	☐	☐
A 6	Is er een globale beschrijving van de werking van het computerprogramma? verwijzing: III/ 3 & IV/ opmerking auditee: opmerking auditor: Toelichting: Geef een overzicht hoe het programma in elkaar zit; welke routines worden gebruikt, waar komen de invoergegevens vandaan, etc. Beschrijf ook hoe het versiebeheer is geregeld en de instellingen van de compiler.	☑	☐	☐
A 7	Zijn alle modelparameters beschreven? verwijzing: III/ 3.4	☑	☐	☐

opmerking auditee:

opmerking auditor:

Toelichting:
Alle modelparameters zijn beschreven, inclusief de herkomst. Maak eventueel ook duidelijk welke parameters door welke experts geschat zijn (expert judgement).

A 8	Is alle invoer beschreven?	☑	☐	☐

verwijzing: IV/

opmerking auditee:

opmerking auditor:

Toelichting:
Beschrijf alle invoer van het programma, inclusief setting- en parameter files die een gebruiker niet ziet.

A 9	Is alle uitvoer beschreven?	☑	☐	☐

verwijzing: IV/

opmerking auditee:

opmerking auditor:

Toelichting:
Beschrijf de uitvoer van het programma, inclusief error-, setting- en parameter files die een gebruiker niet ziet.

Gebruikersdocumentatie
In dit deel wordt het computerprogramma beschreven voor gebruikers. De mate van documentatie is afhankelijk van het soort gebruikers van het model. Dit onderdeel kan worden overgeslagen als het model alleen in de ontwikkelgroep wordt gebruikt. Vraag A16 blijft wel relevant en kan opgenomen worden in de web site of in de samenvatting van de technische documentatie. Het verdient de voorkeur deze documentatie in het engels te schrijven. Kijk op de site "Kwaliteit modellen en bestanden" voor voorbeelden, templates en "handreikingen".

		ja	nee	n.v.t.
A 10	Is het toepassingsgebied van het model beschreven en zijn er voorbeelden van uitgevoerde modelstudies gegeven?	☑	☐	☐

verwijzing: III/ 4.2

opmerking auditee:

opmerking auditor:

Toelichting:

A 11	Is het benodigde kennisniveau van de gebruiker van het model beschreven?	☑	☐	☐

verwijzing: III/ 3.1

opmerking auditee:

opmerking auditor:

Toelichting:
Geef hier het benodigde niveau van zowel de kennis van computers en de gebruikte programmatuur als van de vakinhoudelijke kennis.

A 12	Zijn de beperkingen van het computerprogramma beschreven?	☑	☐	☐

verwijzing: III/ 4.1

opmerking auditee:

opmerking auditor:

Toelichting:
Geef hier de beperkingen van het model op het gebied van de mogelijke toepassingen en de technische beperkingen. Geef ook een lijst met bekende bugs en eventuele work-arounds.

A 13	Is het user interface beschreven? verwijzing: IV/ opmerking auditee: opmerking auditor: Toelichting: Beschrijf het user interface voor een gebruiker indien dit niet direct en intuïtief duidelijk is.	☑	☐	☐
A 14	Is de invoer beschreven? verwijzing: IV/ opmerking auditee: opmerking auditor: Toelichting: Beschrijf de voor de gebruiker relevante invoer van het programma. Geef aandacht aan de eenheden die gebruikt worden.	☑	☐	☐
A 15	Is de uitvoer beschreven? verwijzing: IV/,III/ table 5 opmerking auditee: opmerking auditor: Toelichting: Beschrijf de voor de gebruiker relevante uitvoer van het programma. Geef de gebruikte eenheden bij voorkeur in de uitvoer.	☑	☐	☐
A 16	Is er een korte samenvatting van de validaties, de verificaties, het testen, de gevoeligheidsanalyses en de onzekerheidsanalyses van het computerprogramma? verwijzing: III/ 4.3 opmerking auditee: opmerking auditor: Toelichting: Geef voor een gebruiker een kort overzicht wat er is gedaan om vertrouwen in het model te krijgen. Verwijs eventueel naar de achterliggende rapportage.	☑	☐	☐

Verificatie en testen software
Hier worden de verificatie van de vertaling van het mathematisch model naar het computerprogramma, de uitgevoerde tests en de resultaten daarvan beschreven. Zie **Validatie** voor de inhoudelijke testen.
Kijk op de site "Kwaliteit modellen en bestanden" voor voorbeelden, templates en "handreikingen".

		ja	nee	n.v.t.
A 17	Is er een set testgegevens waarmee de vertaling van de modelvergelijkingen naar de programmacode is geverifieerd? verwijzing: III/ 5 opmerking auditee:	☑	☐	☐

opmerking auditor:

Toelichting:

- Er is een set testgegevens waarmee de vertaling van het mathematisch model naar het computerprogramma is geverifieerd. Denk hierbij aan:
  - een set waarnemingen of
  - analytische oplossingen waarmee invoergegevens worden gegenereerd of
  - een "utopia", d.w.z. een sterk vereenvoudigde wereld die gebruikt wordt om invoergegevens te genereren.
- Nieuwe versies worden getest en vergeleken met een dergelijke standaard set invoergegevens.

A 18 Zijn de meest basale tests op het computerprogramma uitgevoerd? ☑ ☐ ☐

verwijzing: III/ 5

opmerking auditee:

opmerking auditor:

Toelichting:
Voor de gehele code:

- Er is een dimensieanalyse uitgevoerd op alle modelberekeningen.
- Alle code is door een "code checker" (b.v. Forcheck, Lint) getest.
- Niet gedeclareerde gegevens en parameters worden gesignaleerd (implicit none) en krijgen niet automatisch een default de waarde toegewezen.

A 19 Is het rekenhart geheel getest? ☑ ☐ ☐

verwijzing: III/ 5

opmerking auditee:

opmerking auditor:

Toelichting:
Het rekenhart is geheel getest. Denk hierbij aan de volgende tests:

- Een "maximum coverage" test (worden alle regels code minimaal 1 maal doorlopen bij de tests).
- Een random test.
- Verandert de uitvoer voorspelbaar bij een continue verandering van de invoer over het gehele toegestane bereik? (b.v. verandert de uitvoer continu bij een continue verandering van de invoer).
- Is het limietgedrag van alle sub-processen van getest? (b.v. is de verdamping nul indien er geen water aanwezig is)
- Is de volgorde van berekeningen/bewerkingen correct? (b.v. wordt in een iteratief proces de juiste tijdstap gebruikt)
- Worden er onafhankelijke balansen van de belangrijkste modelcomponenten bijgehouden en worden deze gecontroleerd?
- Wordt er tijdens de berekeningen/bewerkingen getest of de variabelen binnen het "normale" bereik blijven?

A 20 Zijn de testgegevens reproduceerbaar opgeslagen? ☑ ☐ ☐

verwijzing: III/ 5.3

opmerking auditee:

opmerking auditor:

Toelichting:
Reproduceerbaar betekent dat de testgegevens in een versiebeheersysteem staan, of dat ze duidelijk vindbaar en identificeerbaar zijn.

A 21	Zijn de uitgevoerde tests beschreven? verwijzing: III/ 5 opmerking auditee: opmerking auditor: Toelichting: De uitgevoerde tests zijn vastgelegd (wie heeft wat gedaan met welke versie en onder welke omstandigheden) in testrapporten. Deze rapportage wordt opgenomen in het versiebeheersysteem of op een andere reproduceerbare wijze opgeslagen (kan elektronisch opgeslagen zijn).	☑	☐	☐

Kalibratie

In dit deel wordt de kalibratie beschreven, indien kalibreren van toepassing is voor het model. Zie het **Handboek Good Modelling Practice** voor de te volgen methode en formulier.
Kalibratie wordt hier opgevat in de ruime betekenis van het op grond van gegevens en expertkennis toekennen van waarden aan de modelparameters, al dan niet met opgave van nauwkeurigheid.

		ja	nee	n.v.t.
A 22	Is het model voor een toepassing gekalibreerd? verwijzing: III/ 6.1 opmerking auditee: opmerking auditor: Toelichting:	☑	☐	☐
A 23	Is de kalibratie beschreven? verwijzing: I/ & III/ 6.1 opmerking auditee: opmerking auditor: Toelichting: De kalibratie is zo beschreven dat deze reproduceerbaar is. De voorkeur gaat uit naar automatische kalibratieprocedures m.b.v. een tool; zoals b.v. met het tool PEST. Leg de gegevens van de uitgevoerde kalibraties vast indien ze ook zinvolle informatie leveren voor nieuwe toepassingen. Denk hierbij o.a. aan waarden van modelparameters.	☑	☐	☐

Validatie

In dit deel worden de validaties voor het toepassingsgebied van het model beschreven (zover mogelijk en redelijk). Zie het **Handboek Good Modelling Practice** voor de te volgen methode en formulier.
Validatie wordt hier opgevat in de ruime betekenis van het kritisch vergelijken van modelresultaten of deelmodelresultaten met veldwaarnemingen of met resultaten van andere modellen.
In het algemeen zal maar een deel van alle mogelijke toepassingen van een model gevalideerd worden. Validatie studies verhogen dus de validatiestatus van een model.

		ja	nee	n.v.t.
A 24	Zijn de uitgevoerde validaties beschreven? verwijzing: III/ 6.2 opmerking auditee: opmerking auditor: Toelichting:	☑	☐	☐

De validatieset is anders dan de kalibratieset.

A 25	Is in deze beschrijving opgenomen wat nog niet is gevalideerd?	☑	☐	☐
	verwijzing: III/ 6.3			
	opmerking auditee:			
	opmerking auditor:			
	Toelichting: Geef in het kort aan welke validaties nog zinvol zijn om te doen, en welke functionaliteit van het model daarmee gevalideerd wordt.			
A 26	Is er een kritische analyse van mogelijke tekortkomingen?	☑	☐	☐
	verwijzing: III/ 6.4			
	opmerking auditee:			
	opmerking auditor:			
	Toelichting: Het gaat hier om een kritische analyse van de validatie resultaten die verklaart worden uit mogelijke tekortkomingen van het model.			

Gevoeligheidsanalyse
In dit deel worden de gevoeligheidsanalyses voor het toepassingsgebied van het model beschreven. Zie het **Handboek Good Modelling Practice** voor de te volgen methodes en formulieren.
Onder gevoeligheidsanalyse wordt verstaan een deterministische analyse die bestudeert hoe één of ander modelresultaat verandert als er iets wordt veranderd aan de parameters of overige invoer van het model.

		ja	nee	n.v.t.
A 27	Zijn voor het toepassingsgebied van het model gevoeligheidsanalyses uitgevoerd?	☑	☐	☐
	verwijzing: III/ 7			
	opmerking auditee:			
	opmerking auditor:			
	Toelichting: Gevoeligheidsanalyses maken mede de sterke en zwakke punten van een model duidelijk. Ook wordt meer duidelijkheid verkregen welke parameters en invoergegevens nauwkeurig bekend moeten zijn en welke niet. Dit is afhankelijk van de soort modelstudie. Kies veel voorkomende situaties voor de gevoeligheidsanalyses.			
A 28	Zijn deze gevoeligheidsanalyses beschreven?	☑	☐	☐
	verwijzing: III/ 7			
	opmerking auditee:			
	opmerking auditor:			
	Toelichting:			

Beheers- en exploitatieplan
Dynamische criteria: In dit deel wordt elk jaar beschreven hoe het model wordt beheerd en geëxploiteerd. De geplande kwaliteitsborging en de geplande verbeteringen van het afgelopen jaar worden geëvalueerd. Verbeteringen worden gepland.
Kijk op de site "Kwaliteit modellen en bestanden" voor voorbeelden en templates.

		ja	nee	n.v.t.

A 29 Is er een beheersplan ? ☑ ☐ ☐

verwijzing: V

opmerking auditee:

opmerking auditor:

Toelichting:
Jaarlijks wordt een beheersplan gemaakt.

A 30 Is het inhoudelijk beheer geregeld? ☑ ☐ ☐

verwijzing: V

opmerking auditee:

opmerking auditor:

Toelichting:
Geregeld betekent hier dat er een aanspreekpunt is en dat er tijd is om het beheer uit te voeren.

A 31 Is het technisch beheer geregeld? ☑ ☐ ☐

verwijzing: V

opmerking auditee:

opmerking auditor:

Toelichting:
Onder technisch beheer wordt ook het versiebeheer verstaan. Geregeld betekent hier dat er een aanspreekpunt is en dat er tijd is om het beheer uit te voeren.

A 32 Is de ondersteuning naar de gebruikers geregeld? ☑ ☐ ☐

verwijzing: V

opmerking auditee:

opmerking auditor:

Toelichting:
Van toepassing in het geval van externe gebruikers (extern = buiten ontwikkelgroep).
Geregeld betekent hier dat er een aanspreekpunt is en dat er tijd is om de ondersteuning uit te voeren.

A 33 Zijn de uitgevoerde verbeteringen gerapporteerd? ☑ ☐ ☐

verwijzing: V

opmerking auditee:

opmerking auditor:

Toelichting:
Evalueer kort de verbeteringen van het afgelopen jaar en geef eventueel aan waarom de uitgevoerde verbeteringen afwijken van de geplande.

A 34 Zijn de geplande verbeteringen voor het model beschreven? ☑ ☐ ☐

verwijzing: V

opmerking auditee:

opmerking auditor:

Toelichting:
Geef een kort overzicht van de geplande verbeteringen voor het komende jaar. Gepland betekend dat de financiering rond is of zeer waarschijnlijk (er bestaat een projectplan en mogelijke financier).

Published documents in the Technical reports series of the Statutory Research Tasks Unit for Nature & the Environment from 2015 onwards.

WOt-technical reports are available from the secretary's office, T 0317 – 48 54 71; E info.wnm@wur.nl
Reports can also be downloaded from www.wur.nl/wotnatuurenmilieu

29	Goossen, C.M., M.A. Kiers (2015). *Mass mapping; State of the art en nieuwe ideeën om bezoekersaantallen in natuurgebieden te meten*
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31	Bijlsma, R.J., A. van Kleunen & R. Pouwels (2014). *Structuur- en functiekenmerken van leefgebieden van Vogelrichtlijn- en Habitatrichtlijnsoorten; Een concept en bouwstenen om leefgebieden op landelijk niveau en gebiedsniveau te beoordelen*
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33	Bijlsma, R.J. & J.A.M. Janssen (2014). *Structuur en functie van habitattypen; Onderdeel van de documentatie van de Habitatrichtlijn artikel 17-rapportage 2013*
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35	Kuindersma, W., F.G. Boonstra, R.A. Arnouts, R. Folkert, R.J. Fontein, A. van Hinsberg & D.A. Kamphorst (2015). *Vernieuwingen in het provinciaal natuurbeleid; Vooronderzoek voor de evaluatie van het Natuurpact.*
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38	Verburg, R.W., R. Michels, L.F. Puister (2015). *Aanpassing Instrumentarium Kosten Natuurbeleid (IKN) aan de typologie van het Subsidiestelsel Natuur en Landschap (SNL)*
39	Commissie Deskundigen Meststoffenwet (2015). *Actualisering methodiek en protocol om de fosfaattoestand van de bodem vast te stellen*
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