6 Dynamic Modelling

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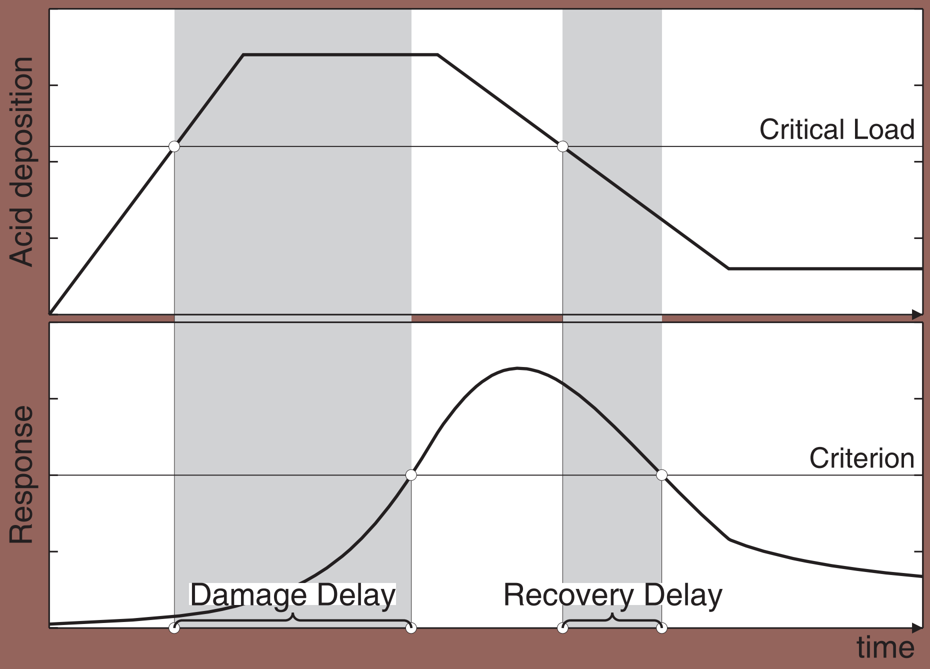

Chapter 6 is an updated version of the Manual for Dynamic Modelling of Soil Response to Atmospheric Deposition, compiled and published by the Coordination Center of Effects in 2003. It has been re-edited by M. Posch and benefited from suggestions made by J. Aherne (Trent University, Ontario, Canada).

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6 Dynamic Modelling

6.1 Introduction

Dynamic modelling is the logical extension of critical loads. Critical loads are based on a steady-state concept, they are the constant depositions an ecosystem can tolerate in the long run, i.e., after it has equilibrated with these depositions. However, many ecosystems are not in equilibrium with present or projected depositions, since there are processes ('buffer mechanisms') at work, which delay the reaching of an equilibrium (steady state) for years, decades or even centuries. By definition, critical loads do not provide any information on these time scales. Dynamic models are needed to assess time delays of recovery in regions where critical loads cease being exceeded and time delays of damage in regions where critical loads continue to be exceeded.

The purpose of this Chapter is to explain the use (and constraints) of dynamic modelling in support of the effects-oriented work under the LRTAP Convention. This Chapter is a shortened and updated version of a 'Dynamic Modelling Manual' published earlier by the CCE (Posch et al. 2003).

For the sake of simplicity and in order to avoid the somewhat vague term 'ecosystem', we refer in the sequel to non-calcareous (forest) soils. However, most of the considerations hold for surface water systems as well, since their water quality is strongly influenced by properties of and processes in catchment soils. A separate report dealing with the dynamic modelling of surface waters on a regional scale has been prepared under the auspices of the ICP Waters (Jenkins et al. 2002).

6.1.1 Why dynamic modelling?

In the causal chain from deposition of strong acids to damage to key indicator organisms there are two major links that can give rise to delays. Biogeochemical processes can delay the chemical response in soil, and biological processes can further delay the response of indicator organisms, such as damage to trees in forest ecosystems. The static models to determine critical loads consider only the steady-state condition, in which the chemical and biological response to a (new) (constant) deposition is complete. Dynamic models, on the other hand, attempt to estimate the time required for a new (steady) state to be achieved.

With critical loads, i.e. in the steady-state situation, only two cases can be distinguished when comparing them to deposition: (1) the deposition is below critical load(s), i.e. does not exceed critical loads, and (2) the deposition is greater than critical load(s), i.e. there is critical load exceedance. In the first case there is no (apparent) problem, i.e. no reduction in deposition is deemed necessary. In the second case there is, by definition, an increased risk of damage to the ecosystem. Thus a critical load serves as a warning as long as there is exceedance, since it states that deposition should be reduced. However, it is often assumed that reducing deposition to (or below) critical loads immediately removes the risk of 'harmful effects', i.e. the chemical criterion (e.g. the Al/Bc-ratio[1]) that links the critical load to the (biological) effect(s), immediately attains a non-critical ('safe') value, and that there is immediate biological recovery as well. But the reaction of soils, especially their solid phase, to changes in deposition is delayed by (finite) buffers, the most important being the cation exchange capacity (CEC). These buffer mechanisms can delay the attainment of a critical chemical parameter, and it might take decades or even centuries, before an equilibrium (steady state) is reached. These finite buffers are not included in the critical load formulation, since they do not influence the steady state, but only the time to reach it. Therefore, dynamic models are needed to estimate the times involved in attaining a certain chemical state in response to deposition scenarios, e.g. the consequences of 'gap closures' in emission reduction negotiations. In addition to the delay in chemical recovery, there is likely to be a further delay before the 'original' biological state is reached, i.e. even if the chemical criterion is met (e.g. Al/Bc<1), it will take time before biological recovery is achieved.

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[1] In Chapter 5 (and elsewhere) the Bc/Al-ratio is used. However, this ratio becomes infinite when the Al concentration approaches zero. To avoid this inconvenience, its inverse, the Al/Bc-ratio, is used here.

Figure 6.1 summarises the possible development of a (soil) chemical and biological variable in response to a ‘typical’ temporal deposition pattern. Five stages can be distinguished:

Stage 1: Deposition was and is below the critical load (CL) and the chemical and biological variables do not violate their respective criteria. As long as deposition stays below the CL, this is the ‘ideal’ situation.

Stage 2: Deposition is above the CL, but (chemical and) biological criteria are not violated because there is a time delay before this happens. No damage is likely to occur at this stage, therefore, despite exceedance of the CL. The time between the first exceedance of the CL and the first violation of the biological criterion (the first occurrence of actual damage) is termed the *Damage Delay Time* $(DDT=t_3-t_1)$.

Stage 3: The deposition is above the CL and both the chemical and biological criteria are violated. Measures (emission reductions) have to be taken to avoid a (further) deterioration of the ecosystem status.

Stage 4: Deposition is below the CL, but the (chemical and) biological criteria are still violated and thus recovery has not yet occurred. The time between the first non-exceedance of the CL and the subsequent non-violation of both criteria is termed the *Recovery Delay Time* $(RDT=t_6-t_4)$.

Stage 5: Deposition is below the CL and both criteria are no longer violated. This stage is similar to Stage 1 and only at this stage can the ecosystem be considered to have recovered.

Stages 2 and 4 can be subdivided into two sub-stages each: Chemical delay times ($DDT_c=t_2-t_1$ and $RDT_c=t_5-t_4$; dark grey in Figure 6.1) and (additional) biological delay times ($DDT_b=t_3-t_2$ and $RDT_b=t_6-t_5$; light grey). Very often, due to the lack of operational biological response models, damage and recovery delay times mostly refer to chemical recovery alone and this is used as a surrogate for overall recovery. It is also important to note that recovery does not follow the same, (inverse) path of damage, since there is a so-called hysteresis in these natural systems (see, e.g., Warfvinge et al. 1992).

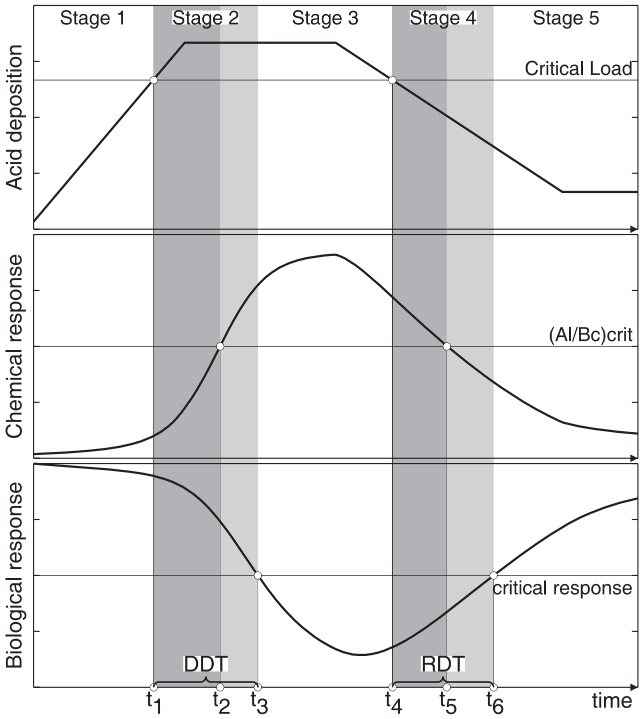

Figure 6.1: ‘Typical’ past and future development of the acid deposition effects on a soil chemical variable (Al/Bc-ratio) and the corresponding biological response in comparison to the critical values of those variables and the critical load derived from them. The delay between the (non)exceedance of the critical load, the (non)violation of the critical chemical criterion and the crossing of the critical biological response is indicated in grey shades, highlighting the Damage Delay Time (DDT) and the Recovery Delay Time (RDT) of the system.

6.1.2 Constraints for dynamic modelling under the LRTAP Convention

Steady-state models (critical loads) have been used to negotiate emission reductions in Europe. In this context, an emission reduction is judged successful if non-exceedance of critical loads is attained. To gain insight into the time delay between the attainment of non-exceedance and actual chemical (and biological) recovery, dynamic models are needed. Thus if dynamic models are to be used to assess recovery under the LRTAP Convention, they should be compatible with the steady-state models used for calculating critical loads. In other words, when critical loads are used as input to the dynamic model, the (chemical) parameter chosen as the criterion in the critical load calculation has to attain the critical value (after the dynamic simulation has reached steady state). But this also means that concepts and equations used in the dynamic model have to be an extension of the concepts and equations employed in deriving the steady-state model. For example, if critical loads are calculated with the Simple Mass Balance (SMB) model (see Chapter 5), this model should be the steady-state version of the dynamic model used (e.g., the VSD model, see below).

Due to a lack of (additional) data, it may be impossible to run dynamic models on all sites in a country for which critical loads have been calculated. The selection of the subset of sites, at which dynamic models are applied, has to be representative enough to allow comparison with results obtained with critical loads.

6.2 Basic Concepts and Equations

Dynamic models of acidification are based on the same principles as steady-state models: The charge balance of the ions in the soil solution, mass balances of the various ions, and equilibrium equations. However, whereas in steady-state models only infinite sources and sinks are considered (such as base cation weathering), the inclusion of the finite sources and sinks of major ions into dynamic models is crucial, since they determine the long-term (slow) changes in soil (solution) chemistry. The three most important processes involving finite buffers and time-dependent sources/sinks are cation exchange, nitrogen retention and sulphate adsorption.

A short description of the models mentioned in this section, such as VSD, MAGIC, SAFE and SMART, can be found in Section 6.3.

6.2.1 Charge and mass balances

As mentioned above, we consider as 'ecosystem' non-calcareous forest soils, although most of the considerations hold also for non-calcareous soils covered by (semi-)natural vegetation. Since we are interested in applications on a large regional scale (for which data are scarce) and long time horizons (decades to centuries with a time step of one year), we make the same simplifying assumption as for the SMB model (see Chapter 5). We assume that the soil is a single homogeneous compartment and its depth is equal to the root zone. This implies that internal soil processes (such as weathering and uptake) are evenly distributed over the soil profile, and all physico-chemical constants are assumed uniform in the whole profile. Furthermore we assume the simplest possible hydrology: The water leaving the root zone is equal to precipitation minus evapotranspiration; more precisely, percolation is constant through the soil profile and occurs only vertically.

As for the SMB model, the starting point is the charge balance of the major ions in the soil water, leaching from the root zone (cf. eq.5.9):

(6.1)

$$SO_{4,le} + NO_{3,le} - NH_{4,le} - BC_{le} + Cl_{le} = H_{le} \\ + Al_{le} - HCO_{3,le} - RCOO_{le} = -ANC_{le}$$

where $BC=Ca+Mg+K+Na$ and $RCOO$ stands for the sum of organic anions. Eq. 6.1 also defines the acid neutralising capacity, ANC.

The leaching term is given by $X_{le}=Q\cdot[X]$ where $[X]$ is the soil solution concentration (eq/m³) of ion X and Q (m/yr) is the water leaving the root zone.

The concentrations $[X]$ of an ion in the soil compartment, and thus its leaching X_{le}, are either obtained from equilibrium equations with $[H]$, such as $[Al]$, $[HCO_3]$ and $[RCOO]$ (see eqs. 5.42, 5.43 and 5.45), or from mass balance equations. The latter describe the change over time of the total amount of ion X per unit area in the soil matrix/soil solution, X_{tot} (eq/m²):

(6.2)

$$\frac{d}{dt}X_{tot}=X_{in}-X_{le}$$

where X_{in} (eq/m²/yr) is the net input of ion X (sources minus sinks, except leaching).

With the simplifying assumptions used in the derivation of the SMB model, the net input of sulphate and chloride is given by their respective deposition:

(6.3)

$$SO_{4,in}=S_{dep} \quad \text{and} \quad Cl_{in}=Cl_{dep}$$

For base cations the net input is given by (Bc=Ca+Mg+K):

(6.4)

$$BC_{in}=BC_{dep}+BC_{w}-Bc_{u}$$

where the subscripts dep, w and u stand for deposition, weathering and net uptake, respectively. Note, that S adsorption and cation exchange reactions are not included here, they are included in X_{tot} and described by equilibrium equations (see below). For nitrate and ammonium the net input is given by:

(6.5)

$$NO_{3,in}=NO_{x,dep}+NH_{4,ni}-NO_{3,i}\\ -NO_{3,u}-NO_{3,de}$$

(6.6)

$$NH_{4,in}=NH_{3,dep}-NH_{4,ni}-NH_{4,i}-NH_{4,u}$$

where the subscripts ni, i and de stand for nitrification, net immobilisation and denitrification, respectively. In the case of complete nitrification one has $NH_{4,in}=0$ and the net input of nitrogen is given by:

(6.7)

$$NO_{3,in}=N_{in}=N_{dep}-N_{i}-N_{u}-N_{de}$$

6.2.2 From steady state (critical loads) to dynamic models

Steady state means there is no change over time in the total amounts of ions involved, i.e. (see eq.6.2):

(6.8)

$$\frac{d}{dt}X_{tot}=0 \quad \Rightarrow \quad X_{le}=X_{in}$$

From eq.6.7 the critical load of nutrient nitrogen, $CL_{nut}(N)$, is obtained by specifying an acceptable N-leaching, $N_{le,acc}$. By specifying a critical leaching of ANC, $ANC_{le,crit}$, and inserting eqs. 6.3, 6.4 and 6.7 into the charge balance (eq. 6.1), one obtains the equation describing the *critical load function* of S and N acidity, from which the three quantities $CL_{max}(S)$, $CL_{min}(N)$ and $CL_{max}(N)$ can be derived (see Chapter 5).

To obtain time-dependent solutions of the mass balance equations, the term X_{tot} in eq. 6.2, i.e. the total amount (per unit area) of ion X in the soil matrix/soil solution system has to be specified. For ions, which do not interact with the soil matrix, X_{tot} is given by the amount of ion X in solution alone:

(6.9)

$$X_{tot}=\Theta\cdot z\cdot[X]$$

where z (m) is the soil depth under consideration (root zone) and Q (m³/m³) is the (annual average) volumetric water content of the soil compartment. The above equation holds for chloride. For every base cation Y participating in cation exchange, Y_{tot} is given by:

(6.10)

$$Y_{tot} = \Theta \cdot z \cdot [Y] + \rho \cdot z \cdot CEC \cdot E_Y$$

where ρ is the soil bulk density (g/cm³), CEC the cation exchange capacity (meq/kg) and E_Y is the exchangeable fraction of ion Y.

The (long-term) changes of the soil N pool are mostly caused by net immobilisation, and N_{tot} is given by:

(6.11)

$$N_{tot} = \Theta \cdot z \cdot [N] + \rho \cdot z \cdot N_{pool}$$

If there is no ad/desorption of sulphate, $SO_{4,tot}$ is given by eq. 6.9. If sulphate adsorption cannot be neglected, it is given by:

(6.12)

$$SO_{4,tot} = \Theta \cdot z \cdot [SO_4] + \rho \cdot z \cdot SO_{4,ad}$$

When the rate of Al leaching is greater than the rate of Al mobilisation by weathering of primary minerals, the remaining part of Al has to be supplied from readily available Al pools, such as Al hydroxides. This causes depletion of these minerals, which might induce an increase in Fe buffering which in turn leads to a decrease in the availability of phosphate (De Vries 1994). Furthermore, the decrease of those pools in podzolic sandy soils may cause a loss in the structure of those soils. The amount of aluminium is in most models assumed to be infinite and thus no mass balance for Al is considered. The SMART model, however, includes an Al balance, and the terms in eq. 6.2 are $Al_{in}=Al_w$, and Al_{tot} is given by:

(6.13)

$$\begin{aligned} Al_{tot} &= \Theta \cdot z \cdot [Al] + \rho \cdot z \cdot CEC \cdot E_{Al} \\ &\quad + \rho \cdot z \cdot Al_{ox} \end{aligned}$$

where Al_{ox} (meq/kg) is the amount of oxalate extractable Al, the pool of readily available Al in the soil.

Inserting these expressions into eq. 6.2 and observing that $X_{le}=Q \cdot [X]$, one obtains differential equations for the temporal development of the concentration of the different ions. Only in the simplest cases can these equations be solved analytically. In general, the mass balance equations are discretised and solved numerically, with the solution algorithm depending on the model builders' preferences.

6.2.3 Finite buffers

Finite buffers of elements in the soil are not included in the derivation of critical loads, since they do not influence the steady state. However, when investigating the state soils over time as a function of changing deposition patterns, these finite buffers govern the long-term (slow) changes in soil (solution) chemistry. In the following we describe the most important ones in turn.

6.2.3.1 Cation exchange

Generally, the solid phase particles of a soil carry an excess of cations at their surface layer. Since electro-neutrality has to be maintained, these cations cannot be removed from the soil, but they can be exchanged against other cations, e.g. those in the soil solution. This process is known as cation exchange; and every soil (layer) is characterised by the total amount of exchangeable cations per unit mass (weight), the so-called cation exchange capacity (CEC, measured in meq/kg). If X and Y are two cations with charges m and n, then the general form of the equations used to describe the exchange between the liquid-phase concentrations (or activities) $[X]$ and $[Y]$ and the equivalent fractions E_X and E_Y at the exchange complex is

(6.14)

$$\frac{E_X^i}{E_Y^j} = K_{XY} \cdot \frac{[X^{m+}]^n}{[Y^{n+}]^m}$$

where K_{XY} is the so-called exchange (or selectivity) constant, a soil-dependent quantity. Depending on the powers i and j different models of cation exchange can be distinguished: For $i=n$ and $j=m$ one obtains the Gaines-Thomas exchange equations, whereas for $i=j=mn$, after taking the mn-th root, the Gapon exchange equations are obtained.

The number of exchangeable cations considered depends on the purpose and complexity of the model. For example, Reuss (1983) considered only the exchange between Al and Ca (or divalent base cations). In general, if the exchange between N ions is considered, $N–1$, exchange equations (and constants) are required, all the other $(N–1)(N–2)/2$ relationships and constants can be easily derived from them. In the VSD, SMART and SAFE model the exchange between aluminium, divalent base cations and protons is considered. The exchange of protons is important, if the cation exchange capacity (CEC) is measured at high pH-values (pH=6.5). In the case of the Bc-Al-H system, the Gaines-Thomas equations read:

(6.15)

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

where $Bc=Ca+Mg+K$, with K treated as divalent. The equation for the exchange of protons against Al can be obtained from eqs. 6.15 by division:

(6.16)

$$\frac{E_H^3}{E_{Al}} = K_{HAl} \cdot \frac{[H^+]^3}{[Al^{3+}]} \quad \text{with} \quad K_{HAl} = \sqrt{K_{HBc}^3 / K_{AlBc}}$$

The corresponding Gapon exchange equations read:

(6.17)

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

Again, the H-Al exchange can be obtained by division (with $k_{HAl}=k_{HBc}/k_{AlBc}$). Charge balance requires that the exchangeable fractions add up to one:

(6.18)

$$E_{Bc} + E_{Al} + E_H = 1$$

The sum of the fractions of exchangeable base cations (here E_{Bc}) is called the *base saturation* of the soil; and it is the time development of the base saturation, which is of interest in dynamic modelling. In the above formulations the exchange of Na, NH_4 (which can be important in high NH_4 deposition areas) and heavy metals is neglected (or subsumed in the proton fraction).

Care has to be exercised when comparing models, since different sets of exchange equations are used in different models. Whereas eqs. 6.15 are used in the SMART model (but with $Ca+Mg$ instead of Bc, K-exchange being ignored in the current version), the SAFE model employs the Gapon exchange equations (eqs. 6.17), however with exchange constants $k'_{X/Y}=1/k_{XY}$. In the MAGIC model the exchange of Al with all four base cations is modelled separately with Gaines-Thomas equations, without explicitly considering H-exchange.

6.2.3.2 Nitrogen immobilisation

In the calculation of critical loads the (acceptable, sustainable) long-term *net* immobilisation (i.e. the difference between immobilisation and mineralisation) is assumed to be constant. However, it is well known, that the amount of N immobilised is (at present) in many cases larger than this long-term value. Thus a submodel describing the nitrogen dynamics in the soil is part of most dynamic models. For example, the MAKEDEP model, which is part of the SAFE model system (but can also be used as a stand-alone routine) describes the N-dynamics in the soil as a function of forest growth and deposition.

According to Dise et al. (1998) and Gundersen et al. (1998) the forest floor C/N-ratios may be used to assess risk for nitrate leaching. Gundersen et al. (1998)

suggested threshold values of >30, 25 to 30, and <25 to separate low, moderate, and high nitrate leaching risk, respectively. This information has been used in several models, such as SMART and MAGIC to calculate nitrogen immobilisation as a fraction of the net N input, linearly depending on the C/N-ratio in the mineral topsoil.

In addition to the long-term constant net immobilisation, $N_{i,acc}$, the net amount of N immobilised is a linear function of the actual C/N-ratio, CN_t, between a prescribed maximum, CN_{max}, and a minimum C/N-ratio, CN_{min}:

(6.19)

$$N_{i,t} = \begin{cases} N_{in,t} & \text{for} \quad CN_t \geq CN_{max} \\ \dfrac{CN_t - CN_{min}}{CN_{max} - CN_{min}} \cdot N_{in,t} & \text{for} \; CN_{min} < CN_t < CN_{max} \\ 0 & \text{for} \quad CN_t \leq CN_{min} \end{cases}$$

where $N_{in,t}$ is the available N (e.g., $N_{in,t}=N_{dep,t}-N_{u,t}-N_{i,acc}$). At every time step the amount of immobilised N is added to the amount of N in the top soil, which in turn is used to update the C/N-ratio. The total amount immobilised at every time step is then $N_i=N_{i,acc}+N_{i,t}$. The above equation states that when the C/N-ratio reaches the minimum value, the annual amount of N immobilised equals the acceptable value $N_{i,acc}$ (see Figure 6.2). This formulation is compatible with the critical load formulation for $t \rightarrow \infty$.

6.2.3.3 Sulphate adsorption

The amount of sulphate adsorbed, $SO_{4,ad}$ (meq/kg), is often assumed to be in equilibrium with the solution concentration and is typically described by a Langmuir isotherm (e.g., Cosby et al. 1986):

(6.20)

$$SO_{4,ad} = \frac{[SO_4]}{S_{1/2} + [SO_4]} \cdot S_{max}$$

where S_{max} is the maximum adsorption capacity of sulphur in the soil (meq/kg) and $S_{1/2}$ the half-saturation concentration (eq/m³).

6.2.4 From soils to surface waters

The processes discussed so far are assumed to occur in the soil solution while it is in contact with the soil matrix. To calculate surface water concentrations it is assumed that the water leaves the soil matrix and is exposed to the atmosphere (Cosby et al. 1985, Reuss and Johnson 1986). When this occurs, excess CO_2 in the water degasses. This shifts the carbonate-bicarbonate equilibria and changes the pH (see eq. 5.43). Surface water concentrations are thus calculated by resolving the system of equations presented above at a lower partial pressure of CO_2 (e.g. mean p_{CO2} of 8·10-4 atm for 37 lakes, Cole et al. 1994) while ignoring exchange reactions, nitrogen immobilisation and sulphate adsorption. Since exchanges with the soil matrix are precluded, the concentration of the base cations and the strong acid anions (SO_4, NO_3 and Cl) will not change as the soil water becomes surface water. As such, ANC is conservative (see eq. 6.1).

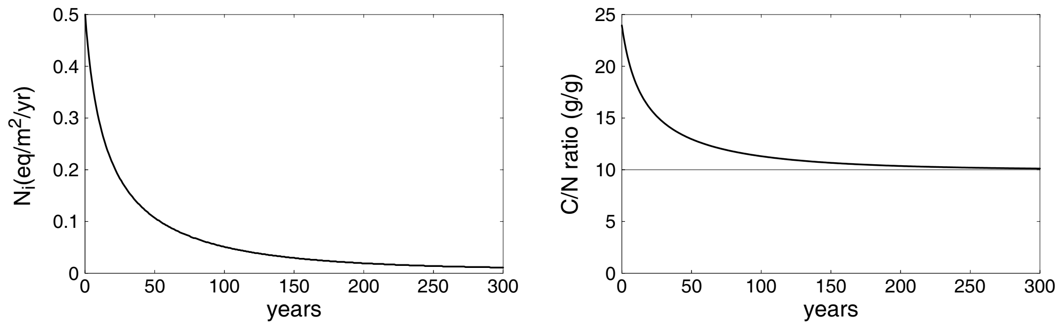

Figure 6.2: Amount of N immobilised (left) and resulting C/N-ratio in the topsoil (right) for a constant net input of N of 1 eq/m²/yr (initial C_{pool} = 4000 gC/m², $N_{i,acc}$ = 1 kg/ha/yr).

6.2.5 Biological response models

Just as there are delays between changes in acid deposition and changes in surface (or soil) water chemistry, there are delays between changes in chemistry and the biological response. Because the goal in recovery is to restore good or healthy population of key indicator organisms, the time lag in response is the sum of the delays in chemical and biological response (see Figure 6.1). Thus dynamic models for biological response are needed; and in the following a summary is provided of existing models and ideas.

6.2.5.1 Terrestrial ecosystems

A major drawback of most dynamic soil acidification models is the neglect of biotic interactions. For example, vegetation changes are mainly triggered by a change in N cycling (N mineralisation; Berendse et al. 1987). Furthermore the enhancement of diseases by elevated N inputs, such as heather beetle outbreaks, may stimulate vegetation changes. Consequently, dynamic soil-vegetation models, which include such processes, have a better scientific basis for the assessment of critical and target N loads. Examples of such models are CALLUNA (Heil and Bobbink 1993) and ERICA (Berendse 1988). The model CALLUNA integrates N processes by atmospheric deposition, accumulation and sod removal, with heather beetle outbreaks and competition between species, to establish the critical N load in lowland dry-heathlands (Heil and Bobbink 1993). The wet-heathland model ERICA incorporates the competitive relationships between the species *Erica* and *Molinia*, the litter production from both species, and nitrogen fluxes by accumulation, mineralisation, leaching, atmospheric deposition and sheep grazing. At present there are also several forest-soil models that do calculate forest growth impacts in response to atmospheric deposition and other environmental aspects, such as meteorological changes (precipitation, temperature) and changes in CO_2 concentration. Examples are the models NAP (Van Oene 1992), ForSVA (Oja et al. 1995) and Hybrid (Friend et al. 1997).

To date, biological dose/response models related to impacts on species diversity in terrestrial ecosystems did not focus on time-dynamic aspects. Instead, statistical models have been developed to assess the relationship between the species diversity of the ecosystem and abiotic aspects related to acidification and eutrophication. An example is the vegetation model MOVE (Latour and Reiling 1993), that predicts the occurrence probability of plant species in response to scenarios for acidification, eutrophication and desiccation. Input to the model comes from the output of the soil model SMART2 (Kros et al. 1995), being an extension of SMART. The SMART2 model predicts changes in abiotic soil factors indicating acidification (pH), eutrophication (N availability) and desiccation (moisture content) in response to scenarios for acid deposition and groundwater abstraction, including the impact of nutrient cycling (litterfall, mineralisation and uptake). MOVE predicts the occurrence probability of ca 700 species as a function of three abiotic soil factors, including nitrogen availability, using regression relationships. Since combined samples of vegetation and environmental variables are rare, the indication values of plant species by Ellenberg (1985) are used to assess the abiotic soil conditions. Deduction of values for the abiotic soil factors from the vegetation guarantees ecological relevance. Combined samples of vegetation with environmental variables are used exclusively to calibrate Ellenberg indication values with quantitative values of the abiotic soil factors. A calibration of these indication values to quantitative values of the abiotic soil factors is necessary to link the soil module to the vegetation module.

A comparable statistical model is the NTM model (Wamelink et al. 2003, Schouwenberg et al. 2000), that was developed to predict the potential conservation value of natural areas. Normally conservation values are calculated on the basis of plant species or vegetation types. As with MOVE, NTM has the possibility to link the vegetation and the site conditions by using plant ecological indicator values. NTM uses a matrix of the habitats of plant species defined on the basis of moisture, acidity and nutrient availability. The model was calibrated using a set of 160,252 vegetation relevees. A value index per plant species was defined on the basis of rarity, decline and international importance. This index was used to determine a conservation value for each relevee. The value per relevee was then assigned to each species in the relevee and regressed on the Ellenberg indicator values for moisture, acidity and nutrient availability (Ellenberg 1985) using a statistical method (P-splines). The model has these three Ellenberg indication values as input for the prediction of the potential conservation value. A potential conservation value is calculated for a combination of the abiotic conditions and vegetation structure (ecotope). Therefore four vegetation types are accounted for, each represented by a submodel of NTM: heathland, grassland, deciduous forest and pine-forest. Use of those models in dynamic modelling assessments is valuable to gain more insight in the effect of deposition scenarios on terrestrial ecosystems.

6.2.5.2 Aquatic ecosystems

As with terrestrial ecosystems, biological dose/response models for surface waters have not generally focussed on the time-dynamic aspects. For example, the relationship between lake ANC and brown trout population status in Norwegian lakes used to derive the critical limit for surface waters is based on synoptic (once in time) surveys of ANC and fish status in a large number of lakes. Similarly the invertebrate indices (Raddum 1999) and diatom response models (Allot et al. 1995, Battarbee et al. 1996) do not incorporate time-dynamic aspects. Additional information on dose/response comes from traditional laboratory studies of toxicity (chronic and acute) and reproductive success.

Information on response times for various organisms comes from studies of recovery following episodes of pollution, for example, salmon population following chemical spill in a river. For salmon full recovery of the population apparently requires about 10 years after the water chemistry has been restored.

There are currently no available time-dynamic process-oriented biological response models for effects of acidification on aquatic and terrestrial organisms, communities or ecosystems. Such models are necessary for a full assessment of the length of time required for recovery of damage from acidification.

There are several types of evidence that can be used to empirically estimate the time delays in biological recovery. The whole-lake acidification and recovery experiments conducted at the Experimental Lakes Area (ELA), north-western Ontario, Canada, provide such information at realistic spatial and temporal scales. These experiments demonstrate considerable lag times between achievement of acceptable water quality following decrease in acid inputs, and achievement of acceptable biological status. The delay times for various organisms are at least several years. In the case of several fish species irreversible changes may have occurred (Hann and Turner 2000, Mills et al. 2000).

A second source of information on biological recovery comes from liming studies. Over the years such studies have produced extensive empirical evidence on rate of response of individual species as well as communities following liming. There has been little focus, however, on the processes involved.

Finally there is recent documentation of recovery in several regions at which acid deposition has decreased in the 1980s and 1990s. Lakes close to the large point-source of sulphur emissions at Sudbury, Ontario, Canada, show clear signs of chemical and biological recovery in response to substantial decreases in emissions beginning in the late 1970s (Keller and Gunn 1995). Lakes in the nearby Killarney Provincial Park (Ontario, Canada) also show clear signs of biological recovery during the past 20 years (Snucins et al. 2001). Here there are several biological factors that influence the rate of biological recovery such as:

(1) fish species composition and density
(2) dispersal factors such as distance to intact population and ability to disperse

(3) existence of resting eggs (for such organisms such as zooplankton)
(4) existence of precluding species – i.e. the niche is filled.

Recently, a workshop held under the auspices of the UNECE reviewed the current knowledge on models for biological recovery in surface waters (see Wright and Lie 2002).

Future work on biological response models must also include consideration of the frequency and severity of harmful episodes, such as pH shocks during spring snowmelt, or acidity and aluminium pulses due to storms with high seasalt inputs. These links between episodic water chemistry and biological response at all levels (organisms, community, and ecosystem) are poorly quantified and thus not yet ready to be incorporated into process-oriented models.

6.3 Available Dynamic Models

In the previous sections the basic processes involved in soil acidification have been summarised and expressed in mathematical form, with emphasis on slow (long-term) processes. The resulting equations, or generalisations and variants thereof, together with appropriate solution algorithms and input-output routines have over the past 15 years been packaged into soil acidification models, mostly known by their (more or less fancy) acronyms.

There is no shortage of soil (acidification) models, but most of them are not designed for regional applications. A comparison of 16 models can be found in a special issue of the journal ‘Ecological Modelling’ (Tiktak and Van Grinsven 1995). These models emphasise either soil chemistry (such as SMART, SAFE and MAGIC) or the interaction with the forest (growth). There are very few truly integrated forest-soil models. An example is the forest model series ForM-S (Oja et al. 1995), which is implemented not in a ‘conventional’ Fortran code, but is realised in the high-level modelling software STELLA.

The following selection is biased towards models which have been (widely) used and which are simple enough to be applied on a (large) regional scale. Only a short description of the models is given, but details can be found in the references cited. It should be emphasised that the term ‘model’ used here refers, in general, to a model system, i.e. a set of (linked) software (and databases) which consists of pre-processors for input data (preparation) and calibration, post-processors for the model output, and – in general the smallest part – the actual model itself.

An overview of the various models is given in Table 6.1 and a short description below. The first three models are soil models of increasing complexity, whereas the MAGIC model is

Table 6.1: Overview of dynamic models that have been (widely) applied on a regional scale.

Model	Essential process descriptions	Layers	Essential model inputs	Contact
VSD	ANC charge balance Mass balances for BC and N (complete nitrification assumed)	One	CL input data + CEC, base saturation C/N-ratio	M Posch
SMART	VSD model + SO_4 sorption Mass balances for $CaCO_3$ and Al Separate mass balances for NH_4 and NO_3, nitrification Complexation of Al with DOC	One	VSD model + S_{max} and $S_{1/2}$ Ca-carbonate, Al_{ox} nitrification fraction, pK values	W de Vries
SAFE	VSD model + Separate weathering calculation, Element cycling by litterfall, Root decay, Mineralisation and root uptake	Several	VSD model + Input data for PROFILE, litterfall rate, parameters describing mineralisation and root uptake	H Sverdrup
MAGIC	VSD model + SO_4 sorption, Al speciation/complexation, Aquatic chemistry	Several (mostly one)	VSD model + S_{max} and $S_{1/2}$ pK values for several Al reactions parameters for aquatic chemistry	RF Wright

generally applied at the catchment level. Application on the catchment level, instead on a single (forest) plot, has implications for the derivation of input data. For example, weathering rates have to represent the average weathering of the whole catchment, data that is difficult to obtain from soil parameters. Thus in MAGIC catchment weathering is calibrated from water quality data.

6.3.1 The VSD model

The basic equations presented in section 6.2 have been used to construct a **V**ery **S**imple **D**ynamic (VSD) soil acidification model. The VSD model is designed as the simplest extension of the SMB model for critical loads. It only includes cation exchange and N immobilisation, and a mass balance for cations and nitrogen as described above, in addition to the equations included in the SMB model. It resembles the model presented by Reuss (1980) which, however, does not consider nitrogen processes.

In the VSD model, the various ecosystem processes have been limited to a few key processes. Processes that are *not* taken into account, are: (i) canopy interactions, (ii) nutrient cycling processes, (iii) N fixation and NH_4 adsorption, (iv) interactions (adsorption, uptake, immobilisation and reduction) of SO_4, (v) formation and protonation of organic anions, $(RCOO)$ and (vi) complexation of Al with OH, SO_4 and $RCOO$.

The VSD model consists of a set of mass balance equations, describing the soil input-output relationships, and a set of equations describing the rate-limited and equilibrium soil processes, as described in section 6.2. The soil solution chemistry in VSD depends solely on the net element input from the atmosphere (deposition minus net uptake minus net immobilisation) and the geochemical interaction in the soil (CO_2 equilibria, weathering of carbonates and silicates, and cation exchange). Soil interactions are described by simple rate-limited (zero-order) reactions (e.g. uptake and silicate weathering) or by equilibrium reactions (e.g. cation exchange). It models the exchange of Al, H and $Ca+Mg+K$ with Gaines-Thomas or Gapon equations. Solute transport is described by assuming complete mixing of the element input within one homogeneous soil compartment with a constant density and a fixed depth. Since VSD is a single layer soil model neglecting vertical heterogeneity, it predicts the concentration of the soil water leaving this layer (the rootzone). The annual water flux percolating from this layer is taken equal to the annual precipitation excess. The time step of the model is one year, i.e. seasonal variations are not considered. The model is available from the CCE website (www.rivm.nl/cce); and a detailed description will be found in Posch and Reinds (2005).

6.3.2 The SMART model

The SMART model (**S**imulation **M**odel for **A**cidification's **R**egional **T**rends) is similar to the VSD model, but somewhat extended and is described in De Vries et al. (1989) and Posch et al. (1993). As with the VSD model, the SMART model consists of a set of mass balance equations, describing the soil input-output relationships, and a set of equations describing the rate-limited and equilibrium soil processes. It includes most of the assumptions and simplifications given for the VSD model; and justifications for them can be found in De Vries et al. (1989). SMART models the exchange of Al, H and divalent base cations using Gaines-Thomas equations. Additionally, sulphate adsorption is modelled using a Langmuir equation (as in MAGIC) and organic acids can be described as mono-, di- or tri-protic. Furthermore, it includes a balance for carbonate and Al; thus allowing the calculation from calcareous soils to completely acidified soils that do not have an Al buffer left. In this respect, SMART is based on the concept of buffer ranges expounded by Ulrich (1981). Recently a description of the complexation of aluminium with organic acids has been included. The SMART model has been developed with regional applications in mind, and an early example of an application to Europe can be found in De Vries et al. (1994).

6.3.3 The SAFE model

The SAFE (**S**oil **A**cidification in **F**orest **E**cosystems) model has been developed at the University of Lund (Warfvinge et al. 1993) and a recent description of the model can be found in Alveteg (1998) and Alveteg and Sverdrup (2002). The main differences to the SMART and MAGIC models are: (a) weathering of base cations is not a model input, but it is modelled with the PROFILE (sub-)model, using soil mineralogy as input (Warfvinge and Sverdrup 1992); (b) SAFE is oriented to soil profiles in which water is assumed to move vertically through several soil layers (usually 4), (c) Cation exchange between Al, H and (divalent) base cations is modelled with Gapon exchange reactions, and the exchange between soil matrix and the soil solution is diffusion limited. The standard version of SAFE does not include sulphate adsorption although a version, in which sulphate adsorption is dependent on sulphate concentration and pH has recently been developed (Martinson et al. 2003).

The SAFE model has been applied to many sites and more recently also regional applications have been carried out for Sweden (Alveteg and Sverdrup 2002) and Switzerland (SAEFL 1998, Kurz et al. 1998, Alveteg et al. 1998).

6.3.4 The MAGIC model

MAGIC (**M**odel of **A**cidification of **G**roundwater **I**n **C**atchments) is a lumped-parameter model of intermediate complexity, developed to predict the long-term effects of acidic deposition on soils and surface water chemistry (Cosby et al. 1985a,b,c, 1986). The model simulates soil solution chemistry and surface water chemistry to predict the monthly and annual average concentrations of the major ions in lakes and streams. MAGIC represents the catchment with aggregated, uniform soil compartments (one or two) and a surface water compartment that can be either a lake or a stream. MAGIC consists of (1) a section in which the concentrations of major ions are assumed to be governed by simultaneous reactions involving sulphate adsorption, cation exchange, dissolution-precipitation-speciation of aluminium and dissolution-speciation of inorganic and organic carbon, and (2) a mass balance section in which the flux of major ions to and from the soil is assumed to be controlled by atmospheric inputs, chemical weathering inputs, net uptake in biomass and losses to runoff. At the heart of MAGIC is the size of the pool of exchangeable base cations in the soil. As the fluxes to and from this pool change over time owing to changes in atmospheric deposition, the chemical equilibria between soil and soil solution shift to give changes in surface water chemistry. The degree and rate of change in surface water acidity thus depend both on flux factors and the inherent characteristics of the affected soils.

The soil layers can be arranged vertically or horizontally to represent important vertical or horizontal flowpaths through the soils. If a lake is simulated, seasonal stratification of the lake can be implemented. Time steps are monthly or yearly. Time series inputs to the model include annual or monthly estimates of: (1) deposition (wet plus dry) of ions from the atmosphere; (2) discharge volumes and flow routing within the catchment; (3) biological production, removal and transformation of ions; (4) internal sources and sinks of ions from weathering or precipitation reactions; and (5) climate data. Constant parameters in the model include physical and chemical characteristics of the soils and surface waters, and thermodynamic constants. The model is calibrated using observed values of surface water and soil chemistry for a specified period.

MAGIC has been modified and extended several times from the original version of 1984. In particular organic acids have been added to the model (version 5; Cosby et al. 1995a) and most recently nitrogen processes have been added (version 7; Cosby et al. 2001).

The MAGIC model has been extensively applied and tested over a 15-year period at many sites and in many regions around the world. Overall, the model has proven to be robust, reliable and useful in a variety of scientific and managerial activities.

6.4 Input Data and Model Calibration

Running a dynamic model is usually the least time- or resource-consuming step in an assessment. It takes more time to interpret model output, but most time-consuming is the acquisition and preparation of input data. Rarely can laboratory or literature data be directly used as model inputs. They have to be pre-processed and interpreted, often with the help of other models. Especially for regional applications not all model inputs are available (or directly usable) from measurements at sites, and interpolations and transfer functions have to be derived and used to obtain the necessary input data. When acquiring data from different sources of information, it is important to keep a record of the 'pedigree', i.e. the entire chain of information, assumptions and (mental) models used to produce a certain number. Also the uncertainty of the data should be assessed, recorded and communicated.

As with critical loads, for the policy support of the effects-oriented work under the LRTAP Convention output of dynamic models will most usefully represent not a particular site, but a larger area, e.g. a forest instead of a single tree stand. Therefore, certain variables should be 'smoothed' to represent that larger area. For example, (projected) growth uptake of nutrients (nitrogen and base cations) should reflect the (projected) average uptake of the forest over that area, and not the succession of harvest and re-growth at a particular spot.

6.4.1 Input data

The input data required to run dynamic models depend on the model, but essentially all of them need the following (minimum) data, which can be roughly grouped into in- and output fluxes, and soil properties. Note that this grouping of the input data depends on the model considered. For example, weathering has to be specified as a (constant) input flux in the SMART and MAGIC model, whereas in the SAFE model it is internally computed from soil properties and depends on the state of the soil (e.g. the pH). Some of the input data are also needed in the SMB model to calculate critical loads, and are described in Chapter 5. This chapter thus focuses on additional data and parameters needed to run dynamic models. The most important soil parameters are the cation exchange capacity *(CEC)*, the base saturation and the exchange (or selectivity) constants describing cation exchange, as well as parameters describing nitrogen retention and sulphate ad/desorption, since these parameters determine the long-term behaviour (recovery) of soils.

Ideally, all input data are directly derived from measurements. This is usually not feasible for regional applications, in which case input data have to be derived from relationships (transfer functions) with basic (map) information. In this chapter we provide information on the input data needed for running the VSD model and thus, by extension, also other models. Descriptions and technical details of the input data for those models can be found in Posch et al. (1993) for the SMART model, in Cosby et al. (1985a) for the MAGIC model and in Alveteg and Sverdrup (2002) for the SAFE model.

In most of the (pedo-)transfer functions presented here, soils – or rather soil groups – are characterised by a few properties, mostly organic carbon and clay content of the mineral soil (see also Figure 6.3) . The organic carbon content, C_{org}, can be estimated as 0.5 or 0.4 times the organic matter content in the humus or mineral soil layer, resp. If C_{org}>15%, a soil is considered a *peat* soil. Mineral soils are called *sand* (or sandy soil) here, if the clay content is below 18% (coarse textured soils; see also Table 5.6), otherwise it is called a *clay* (or clayey/loamy soil). Loess soils are soils with more than 50% $silt$, i.e. $clay+sand$<50% (since $clay+silt+sand$=100%).

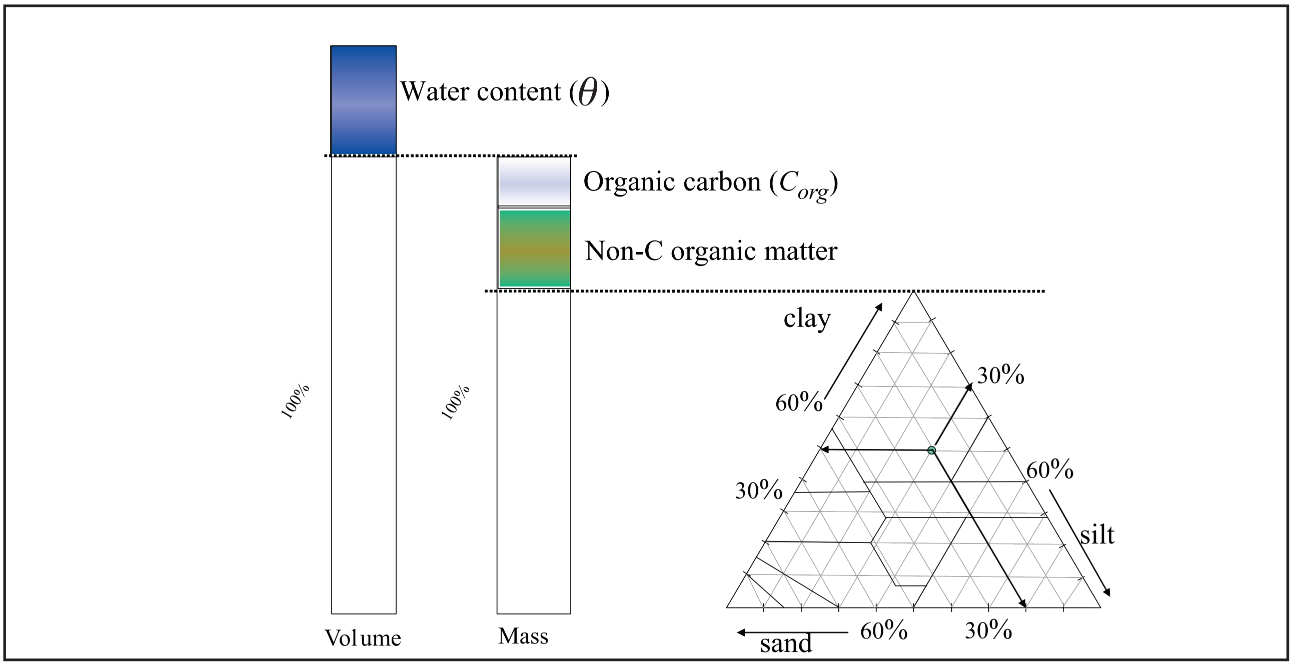

Figure 6.3: Illustration of the basic composition of a soil profile: soil water, organic matter (organic carbon) and the mineral soil, characterised by its *clay*, *silt* and *sand* fraction (*clay*+*silt*+*sand*=100%).

6.4.1.1 Averaging soil properties

For single layer soil models, such as VSD, SMART or MAGIC, the profile averages of certain soil parameters are required, and in the sequel formulae for the average bulk density, cation exchange capacity and base saturation are derived.

For a given soil profile it is assumed that there are measurements of bulk density ρ_l (g/cm³), cation exchange capacity CEC_l (meq/kg) and base saturation $E_{BC,l}$ for n (homogeneous) soil horizons with thickness z_l $(l=1,\ldots,n)$. Obviously, the total thickness (soil depth) z is given by:

(6.21)

$$z=\sum_{l=1}^{n} z_l$$

The mean bulk density ρ of the profile is derived from mass conservation (per unit area):

(6.22)

$$\rho=\frac{1}{z}\sum_{l=1}^{n} z_l\cdot\rho_l$$

The average cation exchange capacity CEC has to be calculated in such a way that the total number of exchange sites (per unit area) is given by $z\cdot\rho\cdot CEC$. This implies the following formula for the profile average cation exchange capacity:

(6.23)

$$CEC=\frac{1}{z\cdot\rho}\sum_{l=1}^{n} z_l\cdot\rho_l\cdot CEC_l$$

And for the profile average base saturation E_{BC} one then gets:

(6.24)

$$E_{BC}=\frac{1}{z\cdot\rho\cdot CEC}\sum_{l=1}^{n} z_l\cdot\rho_l\cdot CEC_l\cdot E_{BC,l}$$

Note that for aquatic ecosystems, these parameters have to be averaged over the terrestrial catchment area as well.

6.4.1.2 Data also used for critical load calculations

In this section we describe those input data which are also used in critical load calculations (see Chapter 5) and for details the reader is referred to that Chapter, especially sections 5.3.1.3 and 5.3.2.3. Whereas for critical loads and exceedance calculations data are needed at a specific point in time (or at steady-state), their past and future temporal development is needed for dynamic modelling.

Deposition:
Non-anthropogenic (steady-state) base cation and chloride deposition are incorporated into the definition of the critical load of acidity. For dynamic models times series of past and future depositions are needed. However, at present there are no projections available for these elements on a European scale. Thus in most model applications (average) present base cation and chloride depositions are assumed to hold also in the future (and past).

Sulphur and nitrogen depositions enter only the exceedance calculations of critical loads. In contrast, their temporal development is the driving force of every dynamic model. Time series for the period 1880-1990 of S and N deposition on the EMEP-150 grid have been recently computed using published estimates of historical emissions (Schöpp et al. 2003) and 12-year average transfer matrices derived from the EMEP/MSC-W lagrangian atmospheric transport model. Scenarios for future sulphur and nitrogen deposition are provided by integrated assessment modellers, based on atmospheric transport modelling by EMEP.

In case the deposition model provides only grid average values, a local deposition (adjustment) model could compute the local deposition from the grid average values, especially for forest soils, where the actual (larger) deposition depends on the type and age of trees (via the 'filtering' of deposition by the canopy). An example of such a model is the MAKEDEP model, which is also part of the SAFE model system (Alveteg and Sverdrup 2002).

Uptake:
Long-term average values of the net growth-uptake of nitrogen and base cations by forests are also needed to calculate critical loads; and data sources and calculation procedures are given in Chapter 5. In simple dynamic models these processes are described as a function of actual and projected forest growth. To this end, additional information on forest age and growth rates is needed, and the amount of data needed depends largely on whether the full nutrient cycle is modelled or whether only net sources and sinks are considered.

Considering net removal by forest growth, as in the VSD, SMART and MAGIC models, the yield (forest growth) at a certain age can be derived from yield tables for the considered tree species. The element contents in stems (and possibly branches) should be the same as used in the critical load calculations (see, e.g., Table 5.2). If the nutrient cycle is modelled, as in the SAFE model, data are needed on litterfall rates, root turnover rates, including the nutrient contents in litter (leaves/needles falling from the tree), and fine roots. Such data are highly dependent on tree species and site conditions. Compilations of such data can be found in De Vries et al. (1990) and Jacobsen et al. (2002).

Water flux and soil moisture:
Water flux data that are needed in one-layer models are limited to the precipitation surplus leaving the root zone (see Chapter 5), whereas multi-layer models require water fluxes for each soil layer down to the bottom of the root zone. For simple dynamic models, water fluxes could be calculated by a separate hydrological model, running on a daily or monthly time step with aggregation to annual values afterwards. An example of such a model is WATBAL (Starr 1999), which is a capacity-type water balance model for forested stands/plots running on a monthly time step and based on the following water balance equation:

(6.25)

$$Q = P - ET \pm \Delta SM$$

where: Q = precipitation surplus, P = precipitation, ET= evapotranspiration and $\pm\Delta SM$ = changes in soil moisture content. WATBAL uses relatively simple input data, which is either directly available (e.g., monthly precipitation and air temperature) or which can be derived from other data using transfer functions (e.g., soil available water capacity).

In any dynamic model, which includes a mass balance for elements, also information on the soil moisture content is needed. This is also output from a hydrological model (see SM in eq. 6.25) or has to be estimated from other site properties. An approximate annual average soil moisture content θ (m³/m³) can be obtained as a function of the clay content (see Brady 1974):

(6.26)

$$\theta = \min\{0.04 + 0.0077 \cdot clay, 0.27\}$$

i.e., for clay contents above 30% a constant value of 0.27 is assumed. It should be noted that most models are quite insensitive to the value of θ.

Base cation weathering:
The various possibilities to assess weathering rates of base cations, which are a key input also to critical load calculations, are discussed and cited in Chapter 5.

Mineralisation and (de-)nitrification:
Rate constants (and possibly additional parameters) for mineralisation, nitrification and denitrification are needed in detailed models, but simple models mostly use factors between zero and one, which compute nitrification and denitrification as fraction of the (net) input of nitrogen.

As in the calculation of critical loads (SMB model), in the VSD model complete nitrification is assumed (nitrification fraction equals 1.0), and denitrification fractions can be found in Table 5.3. Mineralisation is not considered explicitly, but included in the net immobilisation calculations.

For the complete soil profile, the nitrification fraction in forest soils varies mostly between 0.75 and 1.0. This is based on measurements of NH_4/NO_3 ratios below the rootzone of highly acidic Dutch forests with very high NH_4 inputs in the early nineties, which were nearly always less than 0.25 (De Vries et al. 1995). Generally, 50% of the NH_4 input is nitrified above the mineral soil in the humus layer (Tietema et al. 1990). Actually, the nitrification fraction includes the effect of both nitrification and preferential ammonium uptake.

Al-H equilibrium:
The constants needed to quantify the equilibrium between $[Al]$ and $[H]$ in the soil solution are discussed and presented in Chapter 5 (Table 5.9), since they are also needed for critical load calculations. For models including the complexation of Al with organic anions, such as MAGIC and SMART, relevant parameters can be found, e.g., in Driscoll et al. (1994).

6.4.1.3 Data needed to simulate cation exchange

In all dynamic soil models, cation exchange is a crucial process (see section 6.2.3.1). Data needed to allow exchange calculations are:

- The pool of exchangeable cations, being the product of layer thickness, bulk density, cation exchange capacity (CEC) and exchangeable cation fractions
- Cation exchange constants (selectivity coefficients)

Preferably these data are taken from measurements. Such measurements are generally made for several soil horizons. For single-layer models, such as VSD, these data have to be properly averaged over the entire soil depth (rooting zone; see eqs. 6.21 - 6.24).

In the absence of measurements, the various data needed to derive the pool of exchangeable cations for major forest soil types can be derived by extrapolation of point data, using transfer functions between bulk density, CEC and base saturation and basic land and soil characteristics, such as soil type, soil horizon, organic matter content, soil texture, etc.

Soil bulk density:
If no measurements are available, the soil bulk density ρ (g/cm³) can be estimated from the following transfer function:

(6.27)

$$\rho = \begin{cases} 1/\left(0.625 + 0.05 \cdot C_{org} + 0.0015 \cdot clay\right) & \text{for } C_{org} \le 5\% \\ 1.55 - 0.0814 \cdot C_{org} & \text{for } 5\% < C_{org} < 15\% \\ 0.725 - 0.337 \cdot \log_{10} C_{org} & \text{for } C_{org} \ge 15\% \end{cases}$$

where C_{org} is the organic carbon content and *clay* the clay content (both in %). The top equation for mineral soils is based on data by Hoekstra and Poelman (1982), the bottom equation for peat(y) soils is derived from Van Wallenburg (1988) and the central equation is a linear interpolation (for *clay*=0) between the two (Reinds et al. 2001).

Cation exchange capacity (CEC):
The value of the CEC depends on the soil pH at which the measurements are made. Consequently, there is a difference between unbuffered CEC values, measured at the actual soil pH and buffered values measured at a standard pH, such as 6.5 or 8.2. In the VSD (and many other) models the exchange constants are related to a CEC that is measured in a buffered solution in order to standardise to a single pH value (e.g., pH=6.5, as upper limit of non-calcareous soils). The actual CEC can be calculated from pH, clay and organic carbon content according to (after Helling et al. 1964):

(6.28)

$$CEC(pH) = (0.44 \cdot pH + 3.0) \cdot clay \\ + (5.1 \cdot pH - 5.9) \cdot C_{org}$$

where CEC is the cation exchange capacity (meq/kg), *clay* is the clay content (%) and C_{org} the organic carbon content (%). The pH in this equation should be as close as possible to the measured soil solution pH. For sandy soils the clay content can be set to zero in eq. 6.28. Typical average clay contents as a function of the texture class, presented on the FAO soil classification (FAO 1981), are given in Table 6.2. Values for C_{org} range from 0.1% for arenosols (Qc) to 50% for peat soils (Od).

Table 6.2: Average clay contents and typical base saturation as a function of soil texture classes (see Table 5.12).

Texture class	Name	Definition	average clay content (%)	typical base saturation (%)
1	coarse	clay < 18% and sand ≥ 65%	6	5
2	medium	clay < 35% and sand ≥ 15%; but clay ≥ 18% if sand ≥ 65%	20	15
3	medium fine	clay < 35% and sand < 15%	20	20
4	fine	35% ≤ clay < 60%	45	50
5	very fine	clay ≥ 60%	75	50
9	organic soils	Soil types O	5	10-70

Computing $CEC(pH_{measured})$, i.e. the CEC from eq. 6.28, using measured (site-specific) C_{org}, *clay* and pH does not always match the measured CEC, $CEC_{measured}$, and thus computing CEC at pH=6.5, $CEC(6.5)$, would not be consistent with it. Nevertheless, eq. 6.28 can be used to *scale* the measured CEC to a value at $pH=6.5$, i.e. the value needed for modelling, in the following manner:

(6.29)

$$CEC_{pH=6.5} = CEC_{measured} \cdot \frac{CEC(6.5)}{CEC(pH_{measured})}$$

This method of scaling measured data with the ratio (or difference) of model output is widely used in global change work to obtain, e.g., climate-changed (meteorological) data consistent with observations.

<u>Exchangeable base cation fraction (base saturation)</u>:

In most models, a lumped expression is used for the exchange of cations, distinguishing only between H, Al and base cations (VSD, SMART and SAFE). As with the clay content, data for the exchangeable cation fractions, or in some cases only the base saturation, can be based on information on national soil information systems, or in absence of these, on the FAO soil map of Europe (FAO 1981). Base saturation data vary from 5-25% in relatively acid forest soils to more than 50% in well buffered soils. A very crude indication of the base saturation as a function of the texture class of soils is given in the last column of Table 6.2. This relationship is based on data from forest soils given in FAO (1981) and in Gardiner (1987). A higher texture class reflects a higher clay content implying an increase in weathering rate, which implies a higher base saturation. For organic soils the base saturation is put equal to 70% for eutric histosols (Oe) and 10% for dystric histosols (Od).

Ideally, only measured CEC and exchangeable cation data are used. However, when data on the initial base saturation of soils are not available for regional (national) model applications, one may derive them from a relationship with environmental factors. Such an exercise was carried out using a European database with approximately 5300 soil chemistry data for the organic layer and the forest topsoil (0-20 cm) collected on a systematic 16×16 km² grid (ICP Forest level-I grid; Vanmechelen et al. 1997). The regression relationship for the estimated base saturation E_{BC} (expressed as a fraction with values between 0 and 1) is:

(6.30a)

$$E_{BC} = \frac{1}{1+\mathrm{e}^{-B}} \qquad \text{with}$$

(6.30b)

$$\begin{aligned} B = a_0 &+ a_1(\text{soil group}) + a_2(\text{tree species}) + a_3 \cdot \text{altitude} \\ &+ a_4 \cdot \ln(\text{age}) + a_5 \cdot \text{temperature} + a_6 \cdot (\text{temperature})^2 \\ &+ a_7 \cdot \ln(\text{precipitation}) + \sum_{k=8}^{k=11} a_k \cdot \ln(\text{deposition}_k) \\ &+ \sum_{k=12}^{k=15} a_k \cdot \mathrm{lt}(\text{deposition fraction}_k) \end{aligned}$$

where ‘ln’ is the natural logarithm, $lt(x)=ln(x/(1-x))$, and the a_k’s are the regression coefficients. The regression analysis was carried out using a so-called Select-procedure. This procedure combines qualitative predictor variables, such as tree species and/or soil type, with quantitative variables and it combines forward selection, starting with a model including one predictor variable, and backward elimination, starting with a model including all predictor variables. The ‘best’ model was based on a combination of the percentage of explained variance, that should be high and the number of predictor variables that should be low. More information on the procedure is given in Klap et al. (2004). Results of the analyses are given in Table 6.3. The explained variance for base saturation was approx. 45%.

Note: When data are not available, one may also calculate base saturation as the maximum of (i) a relation with environmental factors as given above and (ii) an equilibrium with present deposition levels of SO_4, NO_3, NH_4 and BC. Especially in southern Europe, where acid deposition is relatively low and base cation input is high, the base saturation in equilibrium with the present load can be higher than the value computed according to eq. 6.30.

Table 6.3: Coefficients for estimating base saturation and the *C/N*-ratio in the mineral topsoil (0-20 cm) and the organic layer (after Klap et al. 2004; Note: (a) the star denotes sea-salt corrected depositions, (b) depositions<0.1 should be set to 0.1 to avoid underflow in the equations).

Predictor variable	**Base saturation (mineral topsoil)**	**C/N-ratio (organic layer)**	**C/N-ratio (mineral topsoil)**	**Coefficients in eqs.6.30 and 6.31**
Constant	3.198	3.115	1.310	a_0
Soil group:				
sandy soils	0	0	0	a_1
loamy/clayey soils	0.297	-0.807	-0.279	a_1
peat soils	0.534	-0.025	-0.312	a_1
Tree species:				
pine	0	0	0	a_2
spruce	-0.113	-0.158	-0.093	a_2
oak	0.856	-0.265	-0.218	a_2
beech	0.591	-0.301	-0.218	a_2
Site conditions:				
Altitude [m]	-0.00014	-0.00008	-0.000136	a_3
Age [yr]	0	0.025	0.096	a_4
Meteorology:				
Temperature [°C]	0	-0.0078	-0.041	a_5
Temperature^2 [°C^2]	0	0.00095	0.0014	a_6
Precipitation [mm/yr]	0	0.178	0.194	a_7
Deposition:				
Na [eq/ha/yr]	-0.223	0	0.080	a_8
N-tot (=NO_y+NH_z) [eq/ha/yr]:				
sandy soils	0	-0.150	-0.019	a_9
loamy/clayey soils	0	-0.032	0	a_9
peat soils	0	-0.136	0	a_9
Acid (=SO_x^*+N-tot) [eq/ha/yr]	-1.025	0	0	a_{10}
Bc^* (=Ca^*+Mg^*+K^*) [eq/ha/yr]	0.676	0	0	a_{11}
Deposition fractions:				
NH_z / Acid [-]:				
sandy soils	0	0	0	a_{12}
loamy/clayey soils	-0.494	0	0	a_{12}
peat soils	-0.896	0	0	a_{12}
NH_z /N-tot [-]	0	0.102	0.120	a_{13}
Ca^*/Bc^* [-]	1.211	0	0	a_{14}
Mg^*/Bc^* [-]	0.567	0	0	a_{15}

Exchange constants (selectivity coefficients):
In many exchange models the cations are lumped to *H*, *Al* and base cations (as in VSD, SMART and SAFE), but in MAGIC every base cation (*Ca*, *Mg*, *K*, *Na*) is modelled separately. Furthermore, cation exchange in SMART and MAGIC is based upon Gaines-Thomas equations, in SAFE it is described by Gapon exchange reactions, whereas in the VSD model the user can chose between the two. Exchange constants can be derived from the simultaneous measurement of the major cations (*H*, *Al*, *Ca*, *Mg*, *K* and *Na*) at the adsorption complex and in the soil solution.

Using more than 800 such measurements from Dutch soils, extensive tables of exchange constants have been derived for sand, loess, clay and peat soils, together with their standard deviations and correlations for all combinations of *H*, *Al* and base cations (De Vries and Posch 2003). The data show the high affinity of the complex for protons compared to all other monovalent cations, and that the relative contributions of *K*, *Na* and NH_4 on the adsorption complex are very low. Results for the logarithms ($\log_{10}$) of the exchange constants used in the VSD model, both for the 'Gaines-Thomas mode' and the 'Gapon mode', together with their standard deviation ('stddev') are given in Tables 6.4 to 6.7. For a conversion to other units see Annex III.

Table 6.4: Mean and standard deviation of logarithmic **Gaines-Thomas** exchange constants of H against $Ca+Mg+K$ as a function of soil depth for sand, loess, clay and peat soils (mol/l)$^{-1}$.

Layer	Sand		Loess		Clay		Peat	
(cm)	Mean	stddev	Mean	stddev	Mean	stddev	Mean	stddev
0-10	5.338	0.759	5.322	0.692	6.740	1.464	4.754	0.502
10-30	6.060	0.729	5.434	0.620	6.007	0.740	4.685	0.573
30-60	6.297	0.656	-	-	6.754	0.344	5.307	1.051
60-100	6.204	0.242	5.541	0.579	7.185	-	5.386	1.636
0-30	5.236	0.614	5.386	0.606	6.728	1.373	4.615	0.439
0-60	5.863	0.495	-	-	6.887	1.423	4.651	0.562

Table 6.5: Mean and standard deviation of logarithmic **Gaines-Thomas** exchange constants of Al against $Ca+Mg+K$ as a function of soil depth for sand, loess, clay and peat soils (mol/l).

Layer	Sand		Loess		Clay		Peat	
(cm)	Mean	stddev	Mean	stddev	Mean	stddev	Mean	stddev
0-10	2.269	1.493	1.021	1.147	1.280	1.845	0.835	1.204
10-30	3.914	1.607	1.257	0.939	-0.680	1.152	0.703	0.968
30-60	4.175	1.969	-	-	-3.070	0.298	0.567	1.474
60-100	2.988	0.763	1.652	1.082	-2.860	-	0.969	1.777
0-30	2.306	1.082	0.878	1.079	0.391	1.555	0.978	0.805
0-60	2.858	1.121	-	-	-0.973	1.230	0.666	0.846

Table 6.6: Mean and standard deviation of logarithmic **Gapon** exchange constants of H against $Ca+Mg+K$ as a function of soil depth for sand, loess, clay and peat soils (mol/l)$^{-1/2}$.

Layer	Sand		Loess		Clay		Peat	
(cm)	Mean	stddev	Mean	stddev	Mean	stddev	Mean	stddev
0-10	3.178	0.309	3.138	0.268	3.684	0.568	2.818	0.199
10-30	3.527	0.271	3.240	0.221	3.287	0.282	2.739	0.175
30-60	3.662	0.334	-	-	3.521	0.212	2.944	0.382
60-100	3.866	0.125	3.232	0.251	3.676	-	3.027	0.672
0-30	3.253	0.311	3.170	0.206	3.620	0.530	2.773	0.190
0-60	3.289	0.340	-	-	3.604	0.654	2.694	0.170

Table 6.7: Mean and standard deviation of logarithmic **Gapon** exchange constants of Al against $Ca+Mg+K$ as a function of soil depth for sand, loess, clay and peat soils (mol/l)$^{1/6}$.

Layer	Sand		Loess		Clay		Peat	
(cm)	Mean	stddev	Mean	stddev	Mean	stddev	Mean	stddev
0-10	0.306	0.440	0.190	0.546	-0.312	0.738	-0.373	0.350
10-30	0.693	0.517	0.382	0.663	-0.463	0.431	-0.444	0.255
30-60	0.819	0.527	-	-	-1.476	0.093	-0.740	0.336
60-100	1.114	0.121	0.390	0.591	-1.795	-	-0.867	0.401
0-30	0.607	0.472	0.221	0.647	-0.609	0.731	-0.247	0.404
0-60	0.199	0.633	-	-	-1.054	0.362	-0.551	0.210

It should be noted that exchange constants vary widely and are unknown for most sites. Therefore, in most models (SAFE, MAGIC, but also VSD) they are calibrated against measurements of base saturation (and soil solution concentrations).

6.4.1.4 Data needed for balances of nitrogen, sulphate and aluminium

C/N-ratio:

Data for the C/N-ratio generally vary between 15 in rich soils where humification has been high to 40 in soils with low N inputs and less humification. Values can also be obtained from results of a regression analysis similar to that of the base saturation according to:

(6.31)

$$\ln(\mathrm{C/N\text{-}ratio}) = a_0 + a_1(\mathrm{soil\,group}) + a_2(\mathrm{tree\,species}) + a_3 \cdot \mathrm{altitude} + a_4 \cdot \ln(\mathrm{age}) + a_5 \cdot \mathrm{temperature} + a_6 \cdot (\mathrm{temperature})^2 + a_7 \cdot \ln(\mathrm{precipitation}) + \sum_{k=8}^{k=11} a_k \cdot \ln(\mathrm{deposition}_k) + \sum_{k=12}^{k=15} a_k \cdot \mathrm{lt}(\mathrm{deposition\,fraction}_k)$$

where '*ln*' is the natural logarithm and $lt(x) = ln(x/(1-x))$. Results of the analysis, which was performed with the same data sets as described in the section on base saturation, are given in Table 6.3; and more information on the procedure is given in Klap et al. (2004).

<u>Sulphate sorption capacity and half-saturation constant</u>:
Values for the maximum sorption capacity for sulphate, S_{max}, can be related to the content of oxalate extractable Al (meq kg^{-1}) according to (Johnson and Todd 1983):

(6.32)

$$S_{max} = 0.02 \cdot Al_{ox}$$

Estimates for the oxalate extractable Al content are given below. Adsorption or half-saturation constants for sulphate, $S_{1/2}$, can be derived from literature information (e.g. Singh and Johnson 1986, Foster et al. 1986). A reasonable average value is 1.0 eq/m³.

<u>Al-hydroxide content</u>:
Data for the oxalate extractable Al content (the content of readily available Al-hydroxide) are often available in national soil information systems, such as the soil information system of the Netherlands. In sandy soils the Al-hydroxide content (in meq/kg) mostly varies between 100-200 for A-horizons, between 200-350 for B-horizons and between 50-150 for C-horizons (parent material, De Vries 1991).

6.4.2 Model calibration

If all input parameters, initial conditions and driving forces were known, the chosen model would describe the future development of the soil chemical status for any given deposition scenario. However, in most cases several of the parameters are poorly known, and thus many models, i.e. the badly known parameters in the model, have to be 'calibrated'. The method of calibration varies with the model and/or the application.

In standard applications of both the MAGIC and SAFE model it is assumed that in pre-acidification times (say 1850) the input of ions is in equilibrium (steady state) with the soil (solution) chemistry. Furthermore it is assumed that the deposition history of all (eight) ions is known (properly reconstructed).

In SAFE, weathering rates and uptake/net removal of N and base cations are computed within the model (see above). Only simulated (present) base saturation is matched with observations (in every soil layer) by adjusting the cation exchange selectivity coefficient(s). Matching simulated and observed soil solution concentrations is not part of the standard calibration procedure.

The calibration of MAGIC is a sequential process whereby firstly the input and output of those ions assumed to act conservatively in the catchment are balanced (usually only Cl). Next, the anion concentrations in surface waters are matched by adjusting catchment net retention (of N) and soil adsorption (of S) if appropriate. Thirdly, the four individual major base cation concentration in the stream and on the soil solid phase (expressed as a percentage of cation exchange capacity) are matched by adjusting the cation exchange selectivity coefficients and the base cation weathering rates. Finally, surface water pH, Al and organic anion concentrations are matched by adjusting the aluminium solubility coefficient and total organic acid concentration in surface water.

Both in MAGIC and SAFE automatic calibration routines are an important part of the overall model system. For the SMART model no such automatic model calibration routine is presently available. For the VSD model the same calibration routine as used in SAFE has been implemented, and details can be found in Posch and Reinds (2005) and in the help-file of the 'VSD-Studio' software (available at www.rivm.nl/cce).

6.5 Model Calculations and Presentation of Model Results

As stated above, the most demanding part is not the actual running of a model, but the derivation and preparation of input data (files) and the model initialisation/calibration. However, especially for regional applications, i.e. runs for many sites, additional work is required to embed the model – often designed for single site applications – into a suitable (data base) framework which allows the efficient handling of model inputs and outputs.

6.5.1 Use of dynamic models in integrated assessment

Most usefully, for the review of the Gothenburg Protocol, a link should be established between the dynamic models and integrated assessment (models). In the following several modes of interaction with integrated assessment (IA) models are identified.

Scenario analyses:
Deposition scenario output from IA models are used by the 'effects community' (ICPs) as input to dynamic models to analyse their impact on (European) soils and surface waters, and the results (recovery times etc.) are reported back.

Presently available dynamic models are well suited for this task. The question is how to summarise the resulting information on a European scale. Also, the 'turn-around time' of such an analysis, i.e. the time between obtaining deposition scenarios and reporting back dynamic model results, may be long, as it could involve the work of several subsidiary bodies under the LRTAP Convention.

Response functions:
Response functions are pre-processed dynamic model runs for a large number of plausible future deposition patterns from which the results for every (reasonable) deposition scenario can be obtained by interpolation. Such response functions encapsulate a site's temporal behaviour to reach a certain (chemical) state and linking them to IA models allows to evaluate the site's response to a broad range of deposition patterns.

An example is shown in Figure 6.4: It shows the isolines of years ('recovery isochrones') in which $Al/Bc=1$ is attained for the first time for a given combination of percent deposition reduction (vertical axis) and implementation year (horizontal axis). The reductions are expressed as percentage of the deposition in 2010 after implementation of the Gothenburg Protocol and the implementation year refers to the full implementation of that additional reduction. For example, a 44% reduction of the 2010 deposition, fully implemented by the year 2020 will result in a (chemical) recovery by the year 2040 (dashed line in Figure 6.4). Note that for this example site no recovery is possible, unless deposition is reduced more than 18% of the 2010 level.

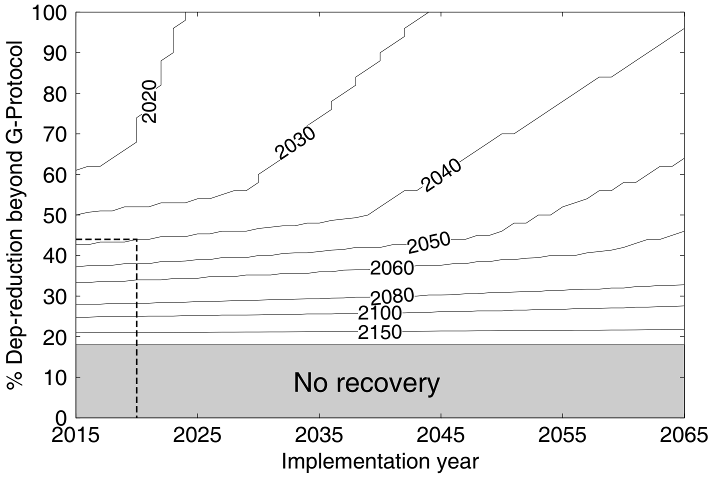

Figure 6.4: Example of 'recovery isochrones' for a single site. The vertical axis gives the additional reduction in acidifying deposition *after* the implementation of the Gothenburg Protocol in 2010 (expressed as percentage of the 2010 level) and the horizontal axis the year at which this additional reductions are fully implemented. The isolines are labelled with the first year at which $Al/Bc=1$ is attained for a given combination of percent reduction and implementation year.

Considering how critical loads have been used in IA during the negotiations of protocols, it is unlikely that there will be a wide variation in the implementation year of a new reduction agreement (generally 5-10 years after a protocol enters into force). Thus, for a fixed implementation year the question will be: What is the maximum deposition allowed to achieve recovery, i.e., reach (and sustain!) a desired chemical state (e.g. $Al/Bc=1$) in a prescribed year? Such a deposition is called a **target load** and, in the case of a single pollutant, target loads can, in principle, be read from information as presented in Figure 6.4. In Figure 6.5 target loads (expressed as percent deposition reductions from the 2010 level) are shown explicitly as function of the target year for the (fixed) implementation year 2020. In the case of a single pollutant, this is the type of information to be linked to IA models.

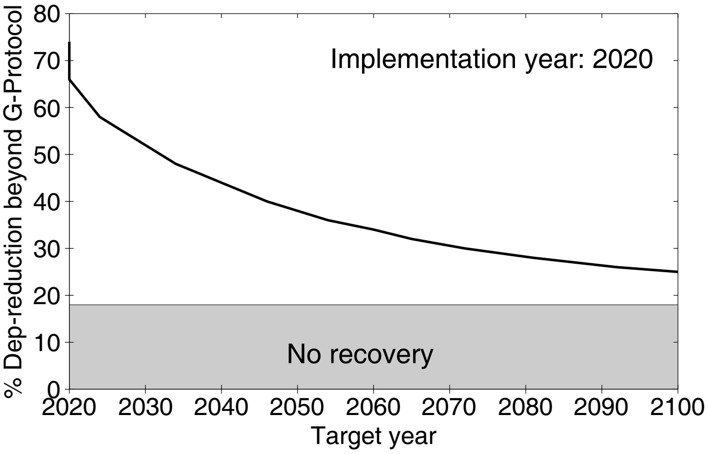

Figure 6.5: Required deposition reductions (target loads) for a site as a function of the target year, i.e. the year in which recovery is achieved (see also Figure 6.4). The implementation year of the reductions is 2020. Note that for reductions above 74% the recovery happens already before the implementation year.

However, in the case of acidity, both N and S deposition determine the soil chemical state and it will not be possible to obtain unique pairs of N and S deposition to reach a prescribed target (similar to critical load functions for acidity). Thus, target loads functions have to be derived with dynamic models for a series of target years and agreed upon implementation years. These target load functions, or suitable statistics derived from them, are passed on to the IA modellers who evaluate their feasibility of achievement (in terms of costs and technological abatement options available).

The determination of response functions, such a target loads, requires no changes to existing models *per se*, but rather additional work, since dynamic soil model have to run many times and/or 'backwards', i.e. in an iterative mode. A further discussion of the problems and possible pitfalls in the computation of target loads is provided in the next section (see also Jenkins et al. 2003).

Integrated dynamic model:
The 'most intimate' link would be the integration of a dynamic model into an IA model (e.g. RAINS). In this way it could be an integral part of all scenario analyses and optimisation runs. Widely used models, such as MAGIC, SAFE and SMART, are not easily incorporated into IA models, and they might be still too complex to be used in optimisation runs. Alternatively, a very simple dynamic model could be incorporated into an IA model, capturing the essential, long-term features of dynamic soil models. This would be comparable to the process that led to the simple ozone model included in RAINS, which was derived from the complex photo-oxidant model of EMEP. However, even this would require a major effort, not the least of which is the creation of a European database to run the model.

6.5.2 Target load calculations

As outlined above, target loads, or target load functions in the case of acidification, are a way to link dynamic models with integrated assessment models, not least due to their similarity with critical load functions (see Chapter 5). If a target load exists, there exists also an infinite variety of deposition paths to reach that target load. To bring order into this multitude and to make results comparable, we define a target load as a deposition path characterised by three numbers (years): (i) the protocol year, (ii) the implementation year, and (iii) the target year (see Figure 6.6). If needed, these terms are proceeded by the term 'dynamic modelling' ('DM') to distinguish them from similar terms used in IA circles.

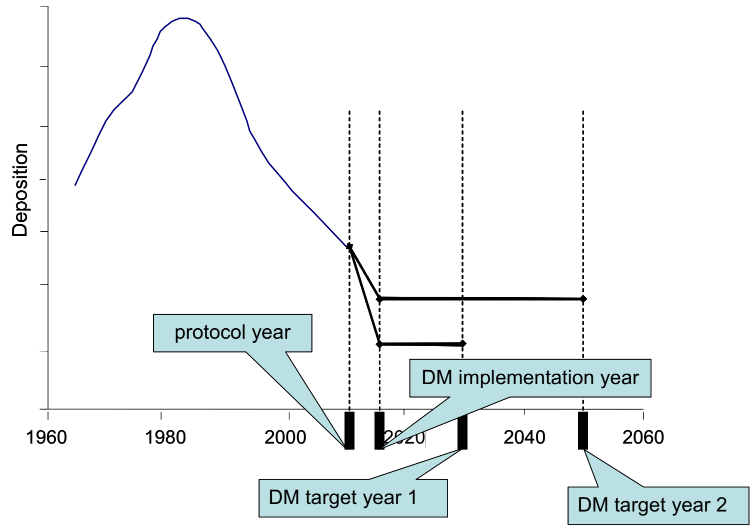

Figure 6.6: Deposition paths for calculating target loads by dynamic models (DM) are characterised by three key years. (i) The year up to which the (historic) deposition is fixed (***protocol year***); (ii) the year in which the emission reductions leading to a target load are fully implemented (***DM implementation year***); and (iii) the years in which the chemical criterion is to be achieved (***DM target years***).

In contrast to scenario analyses, the computation of target loads is not straightforward. After specifying the target year and the year of implementation of the (yet unknown) target load, the dynamic model has to be run iteratively until the deposition (= target load) is found which is required to reach the desired chemical status in the specified target year. The following examples demonstrate the different cases that can arise when calculating target loads and what can happen when doing such calculations 'blindly'. For simplicity we use a single pollutant (deposition), but the conclusions hold for target load functions as well.

As an example, Figure 6.7 shows the deposition history (left) and the resulting molar *Al/Bc*-ratio (right) as simulated (by the VSD model) for three different soils, solely distinguished by their *CEC* (40, 60 and 80 meq/kg). In two cases the *Al/Bc*-ratio in the year 2010 is above the critical value (=1), while for *CEC*=80 it stayed below it during the past. To investigate the future behaviour of the soils, we let the deposition drop to the critical load (which is independent of the *CEC*) during the 'implementation period' (marked by two vertical lines in Figure 6.7). Obviously, for *CEC*=80, the *Al/Bc*-ratio stays below one, whereas for *CEC*=60 it drops below one within the first decade and then slowly rises again towards the critical value. For *CEC*=40, the *Al/Bc*-ratio stays well above the critical value, approaching it asymptotically over time. In all three cases the approach to the critical value is very slow.

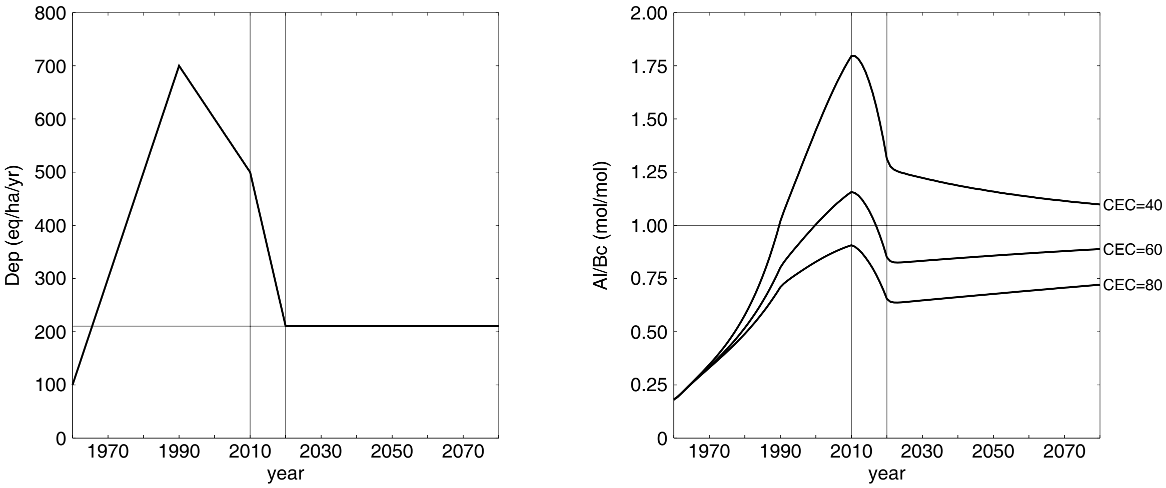

Figure 6.7: Temporal development of acidifying deposition (left) and corresponding molar *Al/Bc*-ratio (right) for 3 soils varying in *CEC*. The two vertical lines separate 50 years of 'history', 10 years (2010-2020) of implementation, and the future. Also shown are the critical load and the critical value $(Al/Bc)_{crit}=1$ as thin horizontal lines. The deposition drops to the critical load within the implementation period and the *Al/Bc*-ratios (slowly) approach the critical value.

Next we look at target load calculations for these three soils. Figure 6.8 shows the results of target load calculations for 40 years, i.e. achieving $(Al/Bc)_{crit}=1$ in the year 2050. For *CEC*=40 meq/kg the target load is smaller than the critical load, as one would expect. For *CEC*=60 and 80, however, the computed target loads are higher than the critical load. As Figure 6.8 illustrates, this does not make sense: After reaching the critical limit, these two soils deteriorate and the *Al/Bc*-ratio gets larger and larger. Since target loads are supposed to protect also *after* the target year, we stipulate that *whenever a calculated target load is higher than the critical load, it has to be set equal to the critical load*.

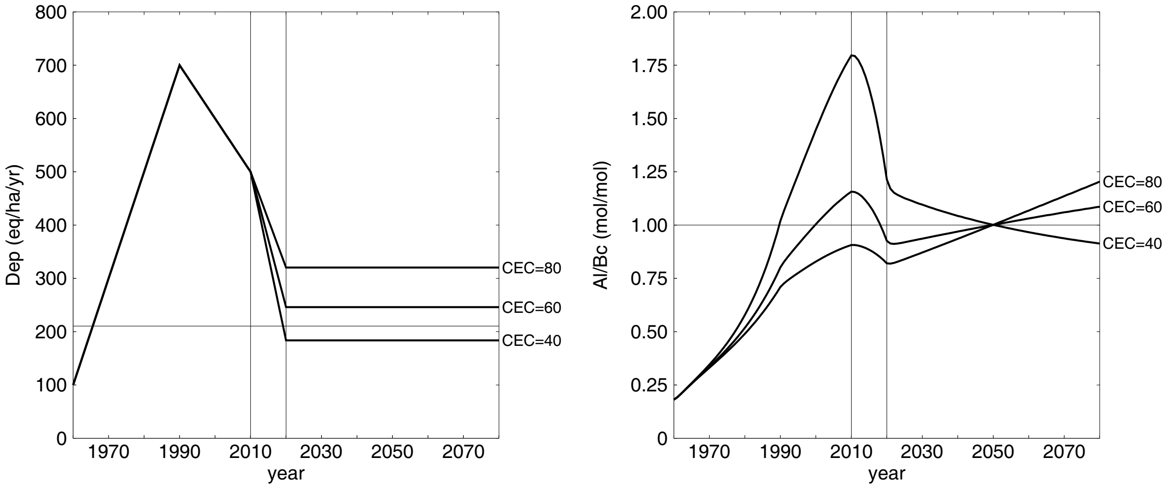

Figure 6.8: Target loads (with 2050 as target year) for three soils and the resulting Al/Bc-ratio (left). Note that for CEC=60 and 80 the target load is higher than the critical load, even when $(Al/Bc)_{crit}<1$ at present (for CEC=80)! Clearly, in such cases target load calculations don't make sense.

In the light of the above considerations we define that ***a target load is the deposition for which a pre-defined chemical or biological status is reached in the target year and maintained (or improved) thereafter.***

In view of this, the steps to be considered for calculating a target load are shown in the flow chart in Figure 6.9. The first check at every site is, whether the critical load (CL) is exceeded in the reference year (2010 in our case). If the answer is 'yes' (as for the soils with CEC=40 and 60 in Figure 6.7), the next step is to run the dynamic model with the deposition equal to the critical load. If in the target year the chemical criterion is no longer violated (e.g. $Al/Bc\leq 1$), the target load equals the critical load $(TL=CL)$.

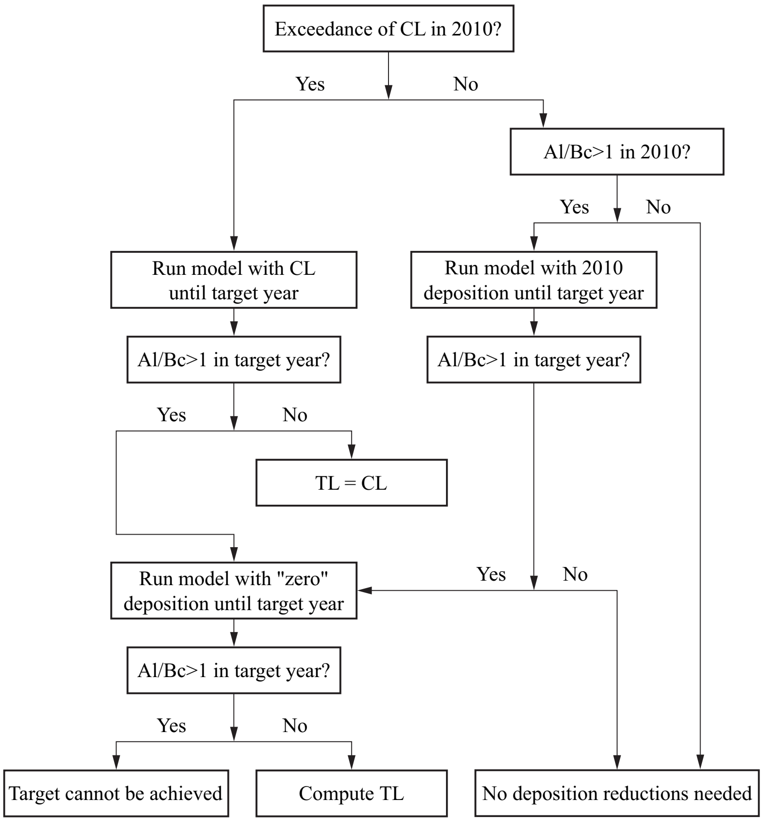

Figure 6.9: Flow chart of the procedure to calculate a target load, avoiding the pitfalls mentioned in the text (e.g. computing a target load that allows violation of the criterion *after* the target year).

If, after running the model with the critical load as deposition, the criterion is still violated in the target year, the model has to be run with "zero" deposition until the specified target year. "Zero" deposition means a deposition small enough as not to contribute to acidification (or eutrophication). In the case of nitrogen this would mean that N_{dep} is set equal to $CL_{min}(N)$, thus avoiding problems, e.g. negatively influencing forest growth in case of zero N deposition.

If, after running the model with "zero" deposition, the criterion is still violated in the target year, then the target cannot be met in that year. In such a case recovery can only be achieved in a later year. Otherwise, a target load exists and has to be calculated; its value lies somewhere between zero and the critical load.

If the critical load is not (or no longer) exceeded in 2010 (as for the soil with CEC=80 in Figure 6.7), this does *not* mean that the risk of damage to the ecosystem is already averted – it only means that *eventually*, maybe after a very long time, the chemical criterion is no longer violated. Only if, in addition, the chemical criterion is not violated in 2010, no further emission reductions are required for that ecosystem. Also, if the model is run with the 2010 deposition until the target year and the criterion is no longer violated in that year, no further emission reductions are required.

In the implementation of the above procedure one could skip the step in which the model is run with the critical load as deposition (in case of exceedance in 2010) and immediately start with target load calculations (if a target load exists). And only afterwards check if this target load is greater than the CL (and set it equal to the CL) (see the soil with CEC=60 in Figure 6.8). However, in view of the fact that TL calculations require iterative model runs, and also to avoid surprises due to round-off errors, it makes good sense to include that intermediate step.

An issue requiring attention in all target load calculations is the assumptions about finite nitrogen buffers. If it is, e.g., assumed that a soil can immobilise N for (say) the next 50 years more than assumed in the critical load calculations, then target loads can be higher than the critical load. This might cause confusion and demands careful explanations.

The above considerations hold also in the case of two pollutants, such as S and N in the case of acidification. The results is then not a single value for a target load, but a so-called **target load function** consisting of all pairs of deposition (N_{dep}, S_{dep}) for which the target is achieved in the selected year. This concept is very similar to the critical load function (see Chapter 5). In Figure 6.10 examples of target load functions are shown or a set of target years.

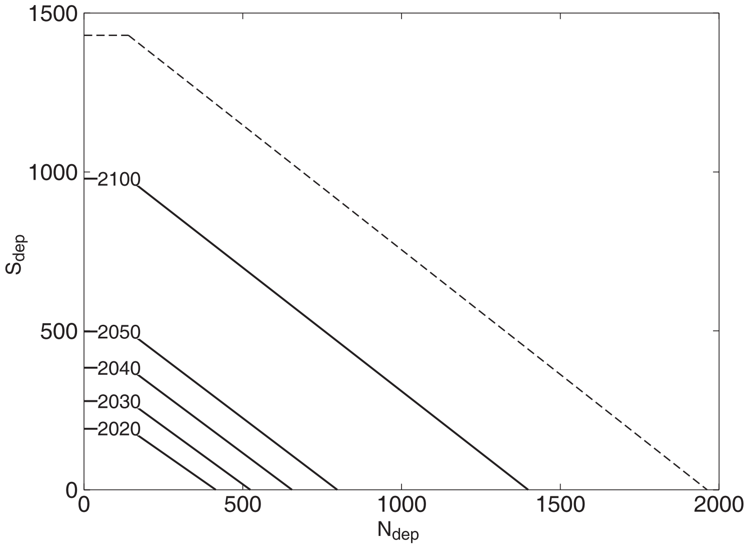

Figure 6.10: Example of target load functions for a site for five different target years. Also shown is the critical load function of the site (dashed line). Note that any meaningful target load function has to lie below the critical load function, i.e. require stricter deposition reductions than achieving critical loads.

When summarising target load calculations for ecosystems in a grid square (or region) it is important not only to report sites for which target load (functions) could been derived, but all cases (and their areas), i.e. the sites for which (i) no further deposition reductions are necessary, (ii) a target load has been calculated, and (iii) no target load exists (for the given target year). Note that in case (i), the 2010 deposition has necessarily to be below (or equal to) the critical load.

6.5.3 Presentation of model results

For single site applications of dynamic models the obvious way to present model output are graphs of the *temporal development of the most relevant soil chemical variables*, such as base saturation or the concentrations of ions in the soil solution (e.g. Al/Bc-ratio), in response to given deposition scenarios. In regional (European) applications, however, this kind of information has to be summarised. This can be done in several ways, e.g., by displaying the temporal development of selected percentiles of the distribution of the variable(s) of interest (see Figure 6.11). Another way is to show a sequence of maps displaying the variable of interest in (say) five-year intervals ('map movies'). These and other options are discussed and illustrated in Evans et al. (2001), Jenkins et al. (2002) and Moldan et al. (2003).

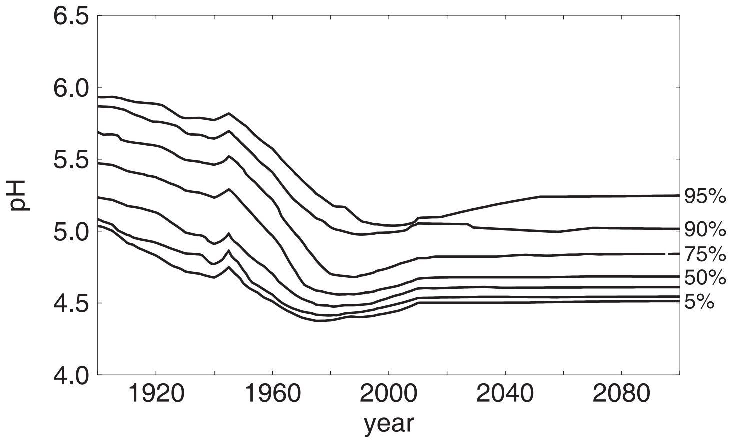

Figure 6.11: Example of percentile traces of a regional dynamic model output. From it seven percentiles (5, 10, 25, 50, 75, 90 and 95%) can be read for every time step.

Maps can represent single sites only if their number does not become too large. If the number of sites reaches the thousands, statistical descriptors (means, percentiles) have to be used to represent the model output. For example, for a given target year the percentage of ecosystems in a grid square for which the target is achieved under a given deposition scenario can be displayed in a map format, very much in the same way as protection percentages (derived from protection isolines) have been displayed for critical load exceedances. Procedures for calculating percentiles and 'target load' isolines can be found in Chapter 8.

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