VII. EXCEEDANCE CALCULATIONS

Updated by Max Posch, CCE, from the initial text of the Mapping Manual 2004
TABLE OF CONTENT

VII. EXCEEDANCE CALCULATIONS ................................................................. 1
VII.1 INTRODUCTION ...................................................................................... 5
VII.2 BASIC DEFINITIONS ............................................................................ 5
VII.3 CONDITIONAL CRITICAL LOADS OF N AND S .................................. 6
VII.4 TWO POLLUTANTS ............................................................................... 7
VII.5 THE AVERAGE ACCUMULATED EXCEEDANCE (AAE) ....................... 10
VII.6 SURFACE WATERS .............................................................................. 11
  VII.6.1 The SSWC model .......................................................................... 11
  VII.6.2 The empirical diatom model ......................................................... 11
  VII.6.3 The FAB model ............................................................................ 11
VII.7 REFERENCES ....................................................................................... 11
VII.1 INTRODUCTION

In this Chapter the calculation of exceedances, i.e. the comparison of critical loads/levels with depositions/concentrations, is described. In Section VII.2 the basic definition of an exceedance is given, including some historical remarks on the origin and use of the word ‘exceedance’. In Section VII.3 the concept of a conditional critical load of S and N is introduced, which allows treating these two acidifying pollutants separately, and thus also makes exceedance calculations straightforward.

VII.2 BASIC DEFINITIONS

The word ‘exceedance’ is defined as "the amount by which something, especially a pollutant, exceeds a standard or permissible measurement" (The American Heritage Dictionary of the English Language, Fourth Edition 2000) and is a generally accepted term within the air pollution discipline. Interestingly, the Oxford English Dictionary (OED) database has an example of ‘exceedance’ from 1836 (Quinion 2004) – 36 years before Robert Angus Smith is credited with coining the term ‘acid rain’ (Smith 1872). However, the term ‘acid rain’ (in French) had already been used in 1845 by Ducros in a scientific journal article (Ducros 1845).

Critical loads and levels are derived to characterise the vulnerability of ecosystem (parts, components) in terms of a deposition or concentration. If the critical load of pollutant X at a given location is smaller than the deposition of X at that location, the critical load is said to be exceeded, and the difference is called exceedance. In mathematical terms, the exceedance $Ex$ of the critical load $CL(X)$ is given as:

$$ Ex(X_{dep}) = X_{dep} - CL(X) $$

where $X_{dep}$ is the deposition of pollutant X. In the case of the critical level, the comparison is with the respective concentration quantity. If the critical load is greater than or equal to the deposition, one says that it is not exceeded or there is non-exceedance of the critical load.

An exceedance defined by eq. VII.1 can obtain positive, negative or zero value. Since it is in most cases sufficient to know that there is non-exceedance, without being interested in the magnitude of non-exceedance, the exceedance can be also defined as:

$$ Ex(X_{dep}) = \max\{0, X_{dep} - CL(X)\} $$

$$ = \begin{cases} X_{dep} - CL(X) & X_{dep} > CL(X) \\ 0 & X_{dep} \leq CL(X) \end{cases} $$

An example of the application of this basic equation is the exceedance of the critical load of nutrient N (see Chapter V), which is given by:

$$ Ex(N_{dep}) = N_{dep} - CL_{nut}(N) $$

In Section VII.4 the exceedance of critical loads is defined that involves two pollutants simultaneously, in Section VII.5 exceedances are regionalised by defining the Average Accumulated Exceedance (AAE), and in Section VII.6 the exceedances of surface water critical loads are considered. Most of the material presented here is based on Posch et al. (1997, 1999, 2001).

1 When comparing deposition(s) to target load (functions), one does not talk about the exceedance, but the ‘non-achievement’ of a target load.

Updated: 16 February 2015
It should be noted that exceedances differ fundamentally from critical loads, as exceedances are time-dependent. One can speak of the critical load of X for an ecosystem, but not of the exceedance of it. For exceedances the time (or the deposition) for which they have been calculated has to be reported, since – especially in integrated assessment – it is exceedances due to (past or future) anthropogenic depositions that are of interest.

Of course, the time-invariance of critical loads and levels has its limitations, certainly when considering a geological time frame. But also during shorter time periods, such as decades or centuries, one can anticipate changes in the magnitude of critical loads due to global (climate) change, which influences the processes from which critical loads are derived. An early example of a study of the (first-order) influence of temperature and precipitation changes on critical loads of acidity and nutrient N in Europe can be found in Posch (2002).

The exceedance of a critical load is often misinterpreted as the amount of excess leaching, i.e. the amount leached above the critical/acceptable leaching. This is in general not the case as exemplified by the exceedance of the critical load of nutrient N. The excess leaching due to the deposition $N_{dep}$, $Ex_{le}$, is given as:

$\text{(VII.4)} \quad Ex_{le} (N_{dep}) = N_{le} - N_{le,acc}$

Inserting the mass balance of N and the deposition-dependent denitrification one obtains for the excess leaching (eqs. V.2–V.5):

$\text{(VII.5)} \quad Ex_{le} (N_{dep}) = (1 - f_{de}) \left( N_{dep} - CL_{max} (N) \right)$

This shows that a deposition reduction of 1 eq/ha/yr reduces the leaching of N by only $1 - f_{de}$ eq/ha/yr. Only in the simplest case, in which all terms of the mass balances are independent of depositions, does the change in leaching equal the change in deposition.

VII.3 CONDITIONAL CRITICAL LOADS OF N AND S

The non-uniqueness of the critical loads of S and N acidity makes both their implementation into integrated assessment models and their communication to decision makers more difficult. However, if one is interested in reductions of only one of the two pollutants, a unique critical load can be derived, and thus also a unique exceedance according to eq. VII.1 can be calculated.

If emission reductions deal with nitrogen only, a unique critical load of N for a fixed sulphur deposition $S_{dep}$ can be derived from the critical load function. We call it the conditional critical load of nitrogen, $CL(N|S_{dep})$, and it is computed as:

$\text{(VII.6)} \quad CL(N | S_{dep}) = \begin{cases} 
CL_{min}(N) & \text{if} \quad S_{dep} \geq CL_{min}(S) \\
CL_{max}(N) - \alpha \cdot S_{dep} & \text{if} \quad S_{dep} < CL_{min}(S)
\end{cases}$

with

$\text{(VII.7)} \quad \alpha = \frac{CL_{max}(N) - CL_{min}(N)}{CL_{max}(S)}$

In Figure VII.1a the procedure for calculating $CL(N|S_{dep})$ is depicted graphically.
Chapter VII – Exceedance calculations

In an analogous manner a conditional critical load of sulphur, $CL(S|N_{dep})$, for a fixed nitrogen deposition $N_{dep}$ can be computed as:

$$CL(S|N_{dep}) = \begin{cases} 0 & \text{if } N_{dep} \geq CL_{max}(N) \\ \frac{CL_{max}(N) - N_{dep}}{\alpha} & \text{if } CL_{min}(N) < N_{dep} < CL_{max}(N) \\ CL_{min}(S) & \text{if } N_{dep} \leq CL_{min}(N) \end{cases}$$

where $\alpha$ is given by eq. VII.7. The procedure for calculating $CL(S|N_{dep})$ is depicted graphically in Figure VII.1b. Setting $N_{dep} = CL_{nut}(N)$, the resulting conditional critical load has been termed minimum critical load of sulphur: $CL_{min}(S) = CL(S|CL_{nut}(N))$.

VII.4 TWO POLLUTANTS

As shown in Chapter V, there is no unique critical load of $N$ and $S$ in the case of acidity or in the case of a critical load function derived from multiple criteria related to $N$ and $S$. Consequently, there is no unique exceedance, although non-exceedance is easily defined (as long as its amount is not important). This is illustrated in Figure VII.2: Let the point E denote the (current) deposition of $N$ and $S$. By reducing $N_{dep}$ substantially, one reaches the point $Z_1$ and thus non-exceedance without reducing $S_{dep}$; on the other hand one can reach non-exceedance by only reducing $S_{dep}$ (by a smaller amount) until reaching $Z_3$; finally, with a reduction of both $N_{dep}$ and $S_{dep}$, one can reach non-exceedance as well (e.g. point $Z_2$).
Figure VII.2: The N-S critical load function defined by two points (four values): \((CLN_{\text{min}}, CLS_{\text{max}})\) and \((CLN_{\text{max}}, CLS_{\text{min}})\). (thick line). The grey-shaded area below the critical load function defines deposition pairs \((N_{\text{dep}}, S_{\text{dep}})\) for which there is no-exceedance. The points \(E\) and \(Z1–Z3\) demonstrate that non-exceedance can be attained in different ways, i.e. there is no unique exceedance.

Intuitively, the reduction required in \(N\) and \(S\) deposition to reach point \(Z_2\) (see Figure VII.2), i.e. the shortest distance to the critical load function, seems a good measure for exceedance. Thus we define the exceedance for a given pair of depositions \((N_{\text{dep}}, S_{\text{dep}})\) as the sum of the \(N\) and \(S\) deposition reductions required to reach the critical load function by the ‘shortest’ path. Figure 7.3 depicts the cases that can arise, if the deposition falls ...

(a) … on or below the critical load function (Region 0). In this case the exceedance is defined as zero (non-exceedance);

(b) … Region 1 (e.g. point \(E_1\)): An \(S\) deposition reduction does not help; an \(N\) deposition reduction is needed: the exceedance is defined as \(N_{\text{dep}}-CL_{\text{max}}N\);

(c) … Region 2 (e.g. point \(E_2\)): the exceedance in this region is defined as the sum of \(N\) and \(S\) deposition reduction needed to reach the corner-point point \(Z_2\);

(d) … Region 3 (e.g. point \(E_3\)): the exceedance is given by the sum of \(N\) and \(S\) deposition reduction, \(ExN+ExS\), required to reach the point \(Z_3\), with the line \(E_3–Z_3\) perpendicular to the CLF;

(e) … Region 4 (e.g. point \(E_4\)): the exceedance is defined as the sum of \(N\) and \(S\) deposition reduction, \(ExN\) and \(ExS\), required to reach the point \(Z_4\);

(f) … Region 5 (e.g. point \(E_5\)): an \(N\) deposition reduction does not help; an \(S\) deposition reduction is needed: the exceedance is defined as \(S_{\text{dep}}-CL_{\text{max}}S\).

Figure VII.3: Illustration of the different cases for calculating the exceedance for a given critical load function.
Chapter VII – Exceedance calculations

The exceedance function can be described by the following equation (the coordinates of the point \( Z_3 \) are denoted by \((N_0, S_0)\); see also Figure VII.2):

\[
(VII.9) \quad \text{Ex}(N_{dep}, S_{dep}) = \begin{cases} 
0 & \text{if } (N_{dep}, S_{dep}) \in \text{Region 0} \\
N_{dep} - CL_{N_{max}} & \text{if } (N_{dep}, S_{dep}) \in \text{Region 1} \\
N_{dep} - CL_{N_{max}} + S_{dep} - CL_{S_{min}} & \text{if } (N_{dep}, S_{dep}) \in \text{Region 2} \\
N_{dep} - N_0 + S_{dep} - S_0 & \text{if } (N_{dep}, S_{dep}) \in \text{Region 3} \\
N_{dep} - CL_{N_{min}} + S_{dep} - CL_{S_{max}} & \text{if } (N_{dep}, S_{dep}) \in \text{Region 4} \\
S_{dep} - CL_{S_{max}} & \text{if } (N_{dep}, S_{dep}) \in \text{Region 5} 
\end{cases}
\]

The function thus defined fulfils the criteria of a meaningful exceedance function: it is zero, if there is non-exceedance, positive when there is exceedance, and increases in value when the point \((N_{dep}, S_{dep})\) moves away from the critical load function.

The computation of the exceedance function requires the estimation of the coordinates of the point \((N_0, S_0)\) on the critical load function. If \((x_1, y_1)\) and \((x_2, y_2)\) are two arbitrary points of a straight line \(g\) and \((x_e, y_e)\) another point (not on that line), then the coordinates \((x_0, y_0) = (N_0, S_0)\) of the point obtained by intersecting the line passing through \((x_e, y_e)\) and perpendicular to \(g\) (called the ‘foot’ or ‘foot of the perpendicular’) are given by:

\[
(VII.10a) \quad x_0 = (d_s + d_x)/d^2 \quad \text{and} \quad y_0 = (d_y - d_x)/d^2
\]

with

\[
(VII.10b) \quad d_1 = x_2 - x_1, \quad d_2 = y_2 - y_1, \quad d^2 = d_1^2 + d_2^2
\]

and

\[
(VII.10c) \quad \begin{cases} 
\Delta = x_1 d_1 + y_1 d_2 \\
\Delta' = x_2 d_1 - y_1 d_2 - x_1 y_2 + y_1 x_2 
\end{cases}
\]

The final difficulty in computing the \(Ex(N_{dep}, S_{dep})\) is to determine into which of the regions (Region 0 through Region 5 in Figure VII.3) a given pair of deposition \((N_{dep}, S_{dep})\) falls. Without going into the details of the geometrical considerations, a FORTRAN subroutine is listed below, which returns the number of the region as well as \(ExN\) and \(ExS\). The correspondences of the 4 quantities – \(CL_{N_{min}}, CL_{S_{max}}, CL_{N_{max}}\) and \(CL_{S_{min}}\) – with the classical critical load function for acidity, defined by \(CL_{max}S\), \(CL_{min}N\) and \(CL_{max}N\), intersected with the nutrient \(N\) critical load \(CL_{nut}(N)\) (or \(CL_{emp}(N)\)) are:

\[
CL_{N_{min}} = CL_{min}N \\
CL_{S_{max}} = CL_{max}S \\
CL_{N_{max}} = CL_{max}N \\
CL_{S_{min}} = CL_{min}N
\]

and, if \(CL_{nut}N < CL_{max}N\):

\[
\begin{cases} 
CL_{max}N = CL_{nut}N \\
CL_{min}N = CL_{max}S \times \frac{CL_{max}N - CL_{nut}N}{CL_{max}N - CL_{min}N}
\end{cases}
\]

otherwise

\[
\begin{cases} 
CL_{N_{max}} = CL_{max}N \\
CL_{S_{min}} = 0
\end{cases}
\]

(see also Posch et al. 2014).

subroutine exceedNS (CLNmin, CLSmax, CLNmax, CLSmin, depN, depS, ExN, ExS, ireg)
!
! Returns the exceedances ExN and ExS (Ex=ExN+ExS) for N and S depositions depN and depS and the CLF defined by (CLNmin,CLSmax) and (CLNmax,CLSmin).
! The "region" in which (depN,depS) lies, is returned in ireg.
!
! implicit none
!
! real, intent(in) :: CLNmin, CLSmax, CLNmax, CLSmin, depN, depS
real, intent(out) :: ExN, ExS
integer, intent(out) :: ireg
!
real :: dN, dS, dd, s, v, xf, yf

Updated: 16 February 2015
Chapter VII – Exceedance calculations

VII.5 THE AVERAGE ACCUMULATED EXCEEDANCE (AAE)

To summarise exceedances in a grid cell (e.g. for mapping) or country/region (for tabulation) one could resort to standard statistical quantities such as mean or any percentile of the distribution of individual exceedance values (see Chapter VIII). Alternatively, the so-called Average Accumulated Exceedance (Posch et al. 2001) has been used, especially in integrated assessment, which is defined as follows.

Let $E_x$ be the exceedance for ecosystem $i$ with area $A_i$, then we define the accumulated exceedance (AE) of $n$ ecosystems on a region (grid cell) as:

\[
AE = \sum_{i=1}^{n} A_i E_x
\]

(VII.11)

For a given deposition, $AE$ is total amount (in eq/yr) deposited in excess over the critical loads in the region in a given year. This function is thus strongly determined by the total ecosystem area in a grid cell. In order to minimise this dependence and to obtain a quantity which is directly comparable to depositions (in eq/ha/yr), we define the average accumulated exceedance (AAE) by dividing the AE function by the total ecosystem area:

\[
AAE = AE / \sum_{i=1}^{n} A_i
\]

(VII.12)

Instead of the total ecosystem area, one could also think of dividing by another area, e.g. the area exceeded for a given (fixed) deposition scenario. However, recalculating the AAE with new areas when depositions change can lead to inconsistencies: the new AAE could be larger, despite declining deposition – as can be shown with simple examples.
VII.6 SURFACE WATERS

Since exceedance calculations for the critical loads for surface waters require special considerations due to the peculiarities of (some of) the models, they are treated here separately. The three critical load models mentioned are described in Chapter V.

VII.6.1 THE SSWC MODEL

In the SSWC model, sulphate is assumed to be a mobile anion (i.e. leaching equals deposition), whereas N is assumed to a large extent to be retained in the catchment by various processes. Therefore, only the so-called present-day exceedance can be calculated from the leaching of N, N_{le}, which is determined from the sum of the measured concentrations of nitrate and ammonia in the runoff. This present exceedance of the critical load of acidity is defined as (Henriksen and Posch 2001):

\[ E(A) = S_{dep} + N_{le} - CL(A) \]

where \( CL(A) \) is the critical load of acidity as computed with eq.V.50. No N deposition data are required for this exceedance calculation; however, \( E(A) \) quantifies only the exceedance at present rates of retention of N in the catchment. Nitrogen processes are modelled explicitly in the FAB model (see below), and thus it is the only surface water model that can be used for comparing the effects of different N deposition scenarios. In the above derivation we assumed that base cation deposition and net uptake did not change over time. If there is increased base cation deposition due to human activities or a change in the net uptake due to changes in management practices, this has to be taken into account in the exceedance calculations by subtracting that anthropogenic \( BC^*_{dep} - Bc_u \) from \( S_{dep} + N_{le} \).

VII.6.2 THE EMPIRICAL DIATOM MODEL

For the diatom model the exceedance of the critical load of acidity is given by:

\[ E(A) = S_{dep} + f_N \cdot N_{dep} - CL(A) \]

VII.6.3 THE FAB MODEL

In the FAB model a critical load function for surface waters is derived in the same way as in the SMB model for soils, and the same considerations hold as given in Section VII.4.

Again there is no unique exceedance for a given pair of depositions \((N_{dep}, S_{dep})\), but an exceedance can be defined in an analogous manner as above (see also Henriksen and Posch 2001).

VII.7 REFERENCES

Ducros M (1845) Observation d'une pluie acide. *Journal de Pharmacie et de Chimie* 3(7): 273-277


Quad M (2004) “The example I quoted [on www.worldwidewords.org] is known to the compilers of the OED (who will be writing an entry for ‘exceedance’ at some point) from their in-house database of unpublished citations. They didn’t provide me with a full citation, only with the date” (personal communication to Julian Aherne in July 2004). – As of January 2014, no entry for ‘exceedance’ had yet been prepared for the OED (email by David Simpson from 25 Jan 2014).