VII. EXCEEDANCE CALCULATIONS

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

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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.

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).

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*[1]. In mathematical terms, the exceedance *Ex* of the critical load *CL*(*X*) is given as:

(VII.1) $$Ex(X_{dep}) = X_{dep} - CL(X)$$

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:

(VII.2)

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

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:

(VII.3) $$Ex_{nut}(N_{dep}) = N_{dep} - CL_{nut}(N)$$

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

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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:

(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):

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

which 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 imple-mentation 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:

(VII.6)

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

with

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

In Figure VII.1a the procedure for calculating $CL(N|S_{dep})$ is depicted graphically.
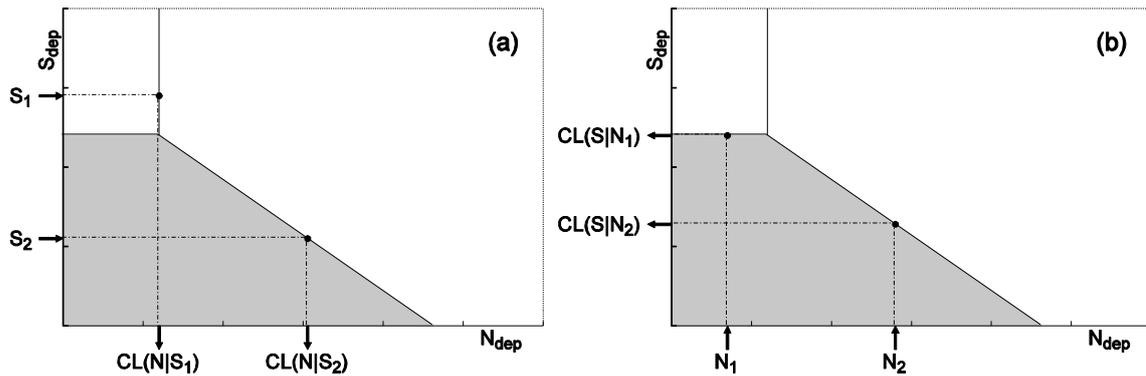
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Figure VII.1: Examples of computing (a) conditional critical loads of N for different S deposition values S1 and S2, and (b) conditional critical loads of S for different N deposition values N1 and N2.

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:

(VII.8)

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

where α 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**: $CL_{min}(S) = CL(S|CL_{nut}(N))$.

When using conditional critical loads, the following caveats should be kept in mind:

(a) A conditional critical load can be considered a true critical load only when the chosen deposition of the other pollutant is kept constant.

(b) If the conditional critical loads of both pollutants are considered simultaneously, care has to be exercised. It is *not* necessary to reduce the exceedances of both, but only one of them to reach non-exceedance for both pollutants; recalculating the conditional critical load of the other pollutant results (in general) in non-exceedance. However, if $S_{dep} > CL_{max}(S)$ or $N_{dep} > CL_{max}(N)$, depositions have to be reduced at least to their respective maximum critical load values, irrespective of the conditional critical loads.

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).
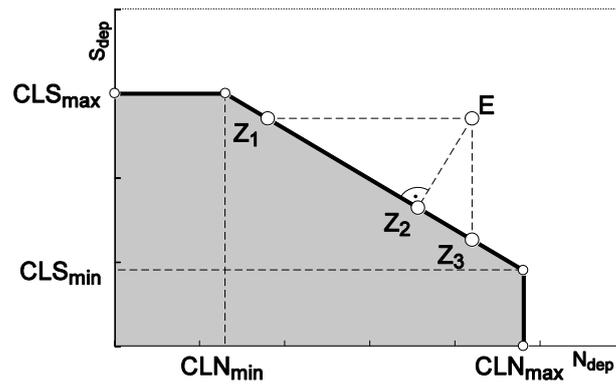
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Figure VII.2 : The N-S critical load function defined by two points (four values): (CLN_{min},CLS_{max}) and (CLN_{max},CLS_{min}). (thick line). The grey-shaded area below the critical load function defines deposition pairs (N_{dep},S_{dep}) for which there is non-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_{dep},S_{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 $N_{dep}-CL_{max}N$;

(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 needed to reach the corner-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 $S_{dep}-CL_{max}S$.
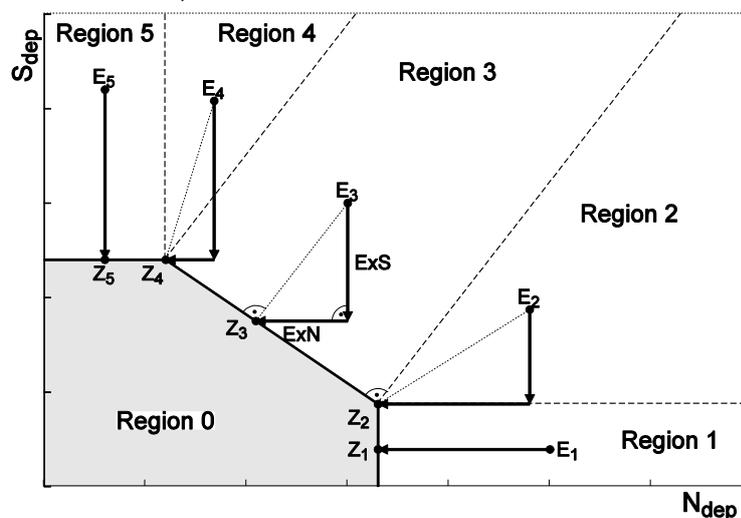

Figure VII.3 : Illustration of the different cases for calculating the exceedance for a given critical load function.

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)

$$Ex(N_{dep}, S_{dep}) = \begin{cases} 0 & \text{if } (N_{dep}, S_{dep}) \in \text{Region } 0 \\ N_{dep} - CLN_{max} & \text{if } (N_{dep}, S_{dep}) \in \text{Region } 1 \\ N_{dep} - CLN_{max} + S_{dep} - CLS_{min} & \text{if } (N_{dep}, S_{dep}) \in \text{Region } 2 \\ N_{dep} - N_0 + S_{dep} - S_0 & \text{if } (N_{dep}, S_{dep}) \in \text{Region } 3 \\ N_{dep} - CLN_{min} + S_{dep} - CLS_{max} & \text{if } (N_{dep}, S_{dep}) \in \text{Region } 4 \\ S_{dep} - CLS_{max} & \text{if } (N_{dep}, S_{dep}) \in \text{Region } 5 \end{cases}$$

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)

$$x_0 = (d_1 s + d_2 v)/d^2 \quad \text{and} \quad y_0 = (d_2 s - d_1 v)/d^2$$

with

(VII.10b)

$$d_1 = x_2 - x_1, \quad d_2 = y_2 - y_1, \quad d^2 = d_1^2 + d_2^2$$

and

(VII.10c)

$$\begin{cases} s = x_e d_1 + y_e d_2, \\ v = x_1 d_2 - y_1 d_1 = x_1 y_2 - y_1 x_2 \end{cases}$$

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 – CLN_{min}, CLS_{max}, CLN_{max} and CLS_{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:

$$CLN_{min} = CL_{min}N$$
$$CLS_{max} = CL_{max}S$$

and, if $CL_{nut}N < CL_{max}N$:

$$\begin{cases} CLN_{max} = CL_{nut}N \\ CLS_{min} = CL_{max}S \times \dfrac{CL_{max}N - CL_{nut}N}{CL_{max}N - CL_{min}N} \end{cases}$$

otherwise

$$\begin{cases} CLN_{max} = CL_{max}N \\ CLS_{min} = 0 \end{cases}$$

(see also Posch et al. 2014).

```fortran
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
```

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```
!
  ExN = -1; ExS = -1; ireg = -1
  if (CLNmin < 0 .or. CLSmax < 0 .or. CLNmax < 0 .or. CLSmin < 0) return
  ExN = depN; ExS = depS; ireg = 9
!  CLN = CLNmax
  if (CLSmax == 0 .and. CLNmax == 0)    return
!  CLS = CLSmin
  dN = CLNmin-CLNmax
  dS = CLSmax-CLSmin
  if (depS <= CLSmax .and. depN <= CLNmax .and. &
&     (depN-CLNmax)*dS <= (depS-CLSmin)*dN) then ! non-exceedance:
    ireg = 0
    ExN = 0; ExS = 0
  else if (depS <= CLSmin) then
    ireg = 1
    ExN = depN-CLNmax; ExS = 0
  else if (depN <= CLNmin) then
    ireg = 5
    ExN = 0; ExS = depS-CLSmax
  else if (-(depN-CLNmax)*dN >=(depS-CLSmin)*dS) then
    ireg = 2
    ExN = depN-CLNmax; ExS = depS-CLSmin
  else if (-(depN-CLNmin)*dN <= (depS-CLSmax)*dS) then
    ireg = 4
    ExN = depN-CLNmin; ExS = depS-CLSmax
  else
    ireg = 3
    dd = dN*dN+dS*dS
    s = depN*dN+depS*dS
    v = CLNmax*dS-CLSmin*dN
    xf = (dN*s+dS*v)/dd
    yf = (dS*s-dN*v)/dd
    ExN = depN-xf; ExS = depS-yf
  end if
                                          return
end subroutine exceedNS
```

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 Ex_i 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:

(VII.11) $$AE = \sum_{i=1}^{n} A_i Ex_i$$

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:

(VII.12) $$AAE = AE / \sum_{i=1}^{n} A_i$$

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, re-calculating 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.

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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):

(VII.13) $Ex(A) = S_{dep} + N_{le} - CL(A)$

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, $Ex(A)$ 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:

(VII.14) $Ex(A) = S_{dep} + f_N \cdot N_{dep} - CL(A)$

where f_N is the fraction of the N deposition contributing to acidification (see eq.V.66).

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).

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VII.7   REFERENCES

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