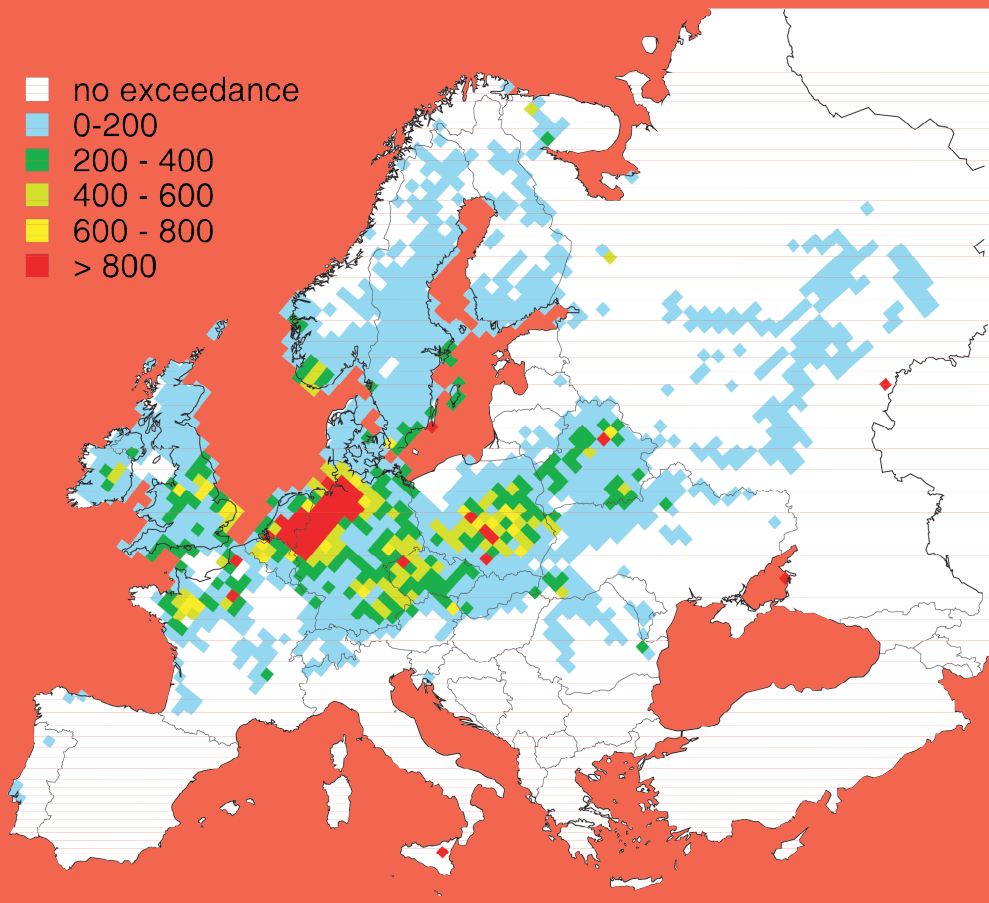
Mapping Manual 2004



This chapter has been compiled by M. Posch, mostly from material scattered in CCE Status Reports. J. Aherne (Canada) read it critically and provided the linguistic information on ‘acid rain’ and ‘exceedance’.

7 Exceedance Calculations

In this Chapter the calculation of exceedances, i.e., the comparison of critical load/levels with depositions/concentrations, is described. In Section 7.1 the basic definition of an exceedance is given, including some historical remarks on the origin and use of the word 'exceedance'. In Section 7.2 the concept of a conditional critical load of S and N is introduced, which allows to treat these two acidifying pollutants separately, and thus also straight-forward exceedance calculations. In Section 7.3 the exceedance of critical loads of acidity is defined, which involves two pollutants simultaneously, in Section 7.4 the exceedances of surface water critical loads are considered, and in Section 7.5 the relationship between depositions and target loads are briefly touched. Most of the material presented here is taken from Posch et al. (1997, 1999).

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. Nevertheless, the term 'critical load excess' is preferred by some (English) speakers due to the apparent coining of 'exceedance' during the development of the critical load concept. 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 of 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).

7.1 Basic Definitions

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, it is said that the critical load is exceeded and the difference is called ***exceedance***. In mathematical terms, the exceedance Ex of the critical load $CL(X)$ is given as:

(7.1)

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

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. 7.1 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:

(7.2)

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

An example of the application of this basic equation is the exceedance of the critical load of nutrient N (see Chapter 5.3.1), which is given by:

(7.3)

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

It should be noted that exceedances differ fundamentally from critical loads, as they 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 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 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:

(7.4)

$$Ex_{le}(N_{dep}) = N_{le} - N_{le,acc}$$

Inserting the mass balance of N and the deposition-dependent denitrification one obtains for the excess leaching (eqs.5.2-5.5):

(7.5)

$$\begin{aligned} Ex_{le}(N_{dep}) &= (1-f_{de}) \cdot \left(N_{dep} - CL_{nut}(N)\right) \\ &= (1-f_{de}) \cdot Ex_{nut}(N_{dep}) \end{aligned}$$

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, equals the change in leaching the change in deposition.

7.2 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. 7.1 can be calculated.

If emission reductions deal with nitrogen only, a unique critical load of N for a fixed sulphur deposition Sdep 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:

(7.6)

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

with

(7.7)

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

In Figure 7.1a the procedure for calculating $CL(N|S_{dep})$ is depicted graphically.

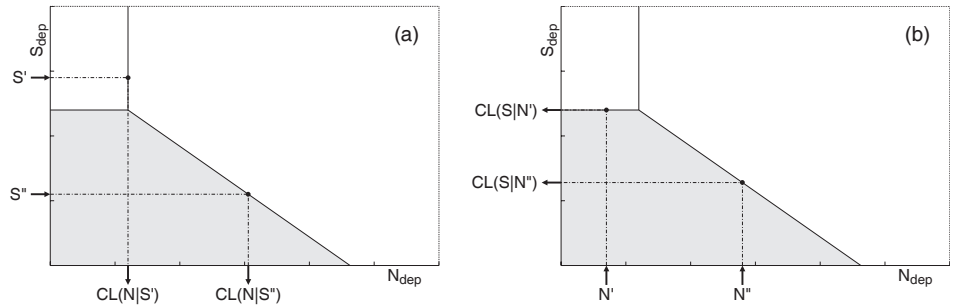


Figure 7.1: Examples of computing (a) conditional critical loads of N for different S deposition values S' and S'', and (b) conditional critical loads of S for different N deposition values N' and N''.

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

(7.8)

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

where α is given by eq. 7.7. The procedure for calculating $CL(N|S_{dep})$ is depicted graphically in Figure 7.1b. Setting N_{dep}=$CL_{nut}(N)$, the resulting conditional critical load has been termed **minimum critical load of sulphur:** $CL_{min}(S)$=$CL(S|CL_{nut}(N))$.

Eq. 7.8 would have been the consistent procedure for calculating critical loads of S used in the negotiations of the 1994 Oslo Protocol; however, critical loads for nitrogen - $CL_{min}(N)$ and $CL_{max}(N)$ - were not available then.

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.

7.3 Two Pollutants

As has been shown in Chapter 5.3, their is no unique critical load of S and N acidity, and all deposition pairs (N_{dep},S_{dep}) lying on the critical load function lead to the critical leaching on ANC (see eq. 5.19 and Figure 5.1). Whereas non-exceedance is easily defined (as long as its amount is not important), there is no unique exceedance of acidity critical loads. This is illustrated in Figure 7.1a: Let the point E denote the (current) deposition of N and S. By reducing N_{dep} substantially, one reaches the point $Z1$ 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 $Z3$; finally, with a reduction of both N_{dep} and S_{dep}, one can reach non-exceedance as well (e.g. point $Z2$).

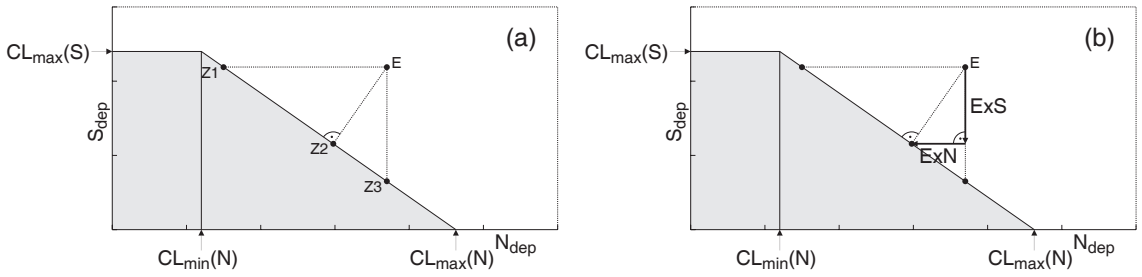


Figure 7.2: Critical load function for S and acidifying N (thick line; see Figure 5.1). The grey-shaded area below the critical load function defines deposition pairs (N_{dep}, S_{dep}) for which there is non-exceedance. (a) The points E and $Z1$-$Z3$ show that there is no unique exceedance; (b) the quantities involved in the definition of an exceedance (see text for further explanations).

Intuitively, the reduction required in N and S deposition to reach point $Z2$ (see Figure 7.2b), 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 five cases that can arise:

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

(b) the deposition falls into Region 1 (e.g. point $E1$). In this case the line perpendicular to the critical load function would yield a negative S_{dep}, and thus every exceedance in this region is defined as the sum of N and S deposition reduction needed to reach point $Z1$;

(c) the deposition falls into Region 2 (e.g. point $E2$): this is the 'regular' case, the exceedance is given by the sum of N and S deposition reduction, $ExN+ExS$, required to reach the point $Z2$, such that the line $E2$-$Z2$ is perpendicular to the critical load function;

(d) Region 3: every exceedance is defined as the sum of N and S deposition reduction needed to reach point $Z3$;

(e) Region 4: the exceedance is simply defined as $S_{dep}–CL_{max}(S)$.

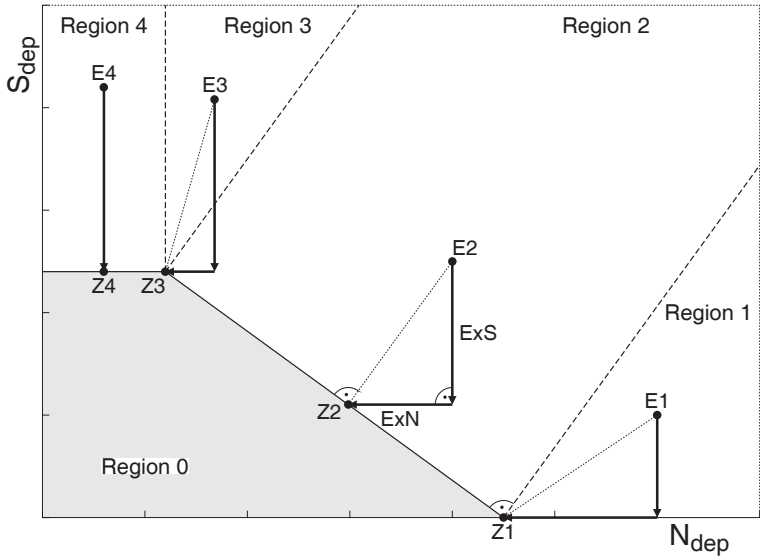


Figure 7.3: Illustration of the different cases for calculating the exceedance for a given critical load function.

The exceedance function can be described by the following equation; note the point $Z2$ on the critical load function obtained by drawing a perpendicular line through a point in Region 2 (see Figure 7.3) is denoted by (N_0, S_0):

(7.9)

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

The function thus defined fulfils the criteria of a meaningful exceedance function: it is zero, if there is no exceedance of critical loads, positive when there is exceedance, and increasing 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 *Z2* 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,x_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:

(7.10a)

$$x_0 = (d_1 s + d_2 v)/d^2 \quad and$$

$$y_0 = (d_2 s - d_1 v)/d^2$$

with

(7.10b)

$$d_1 = x_2 - x_1, \quad d_2 = y_2 - y_1,$$

$$d^2 = d_1^2 + d_2^2$$

and

(7.10c)

$$s = x_e d_1 + y_e d_2,$$

$$v = x_1 d_2 - y_1 d_1 = x_1 y_2 - y_1 x_2$$

Applying these equations to $(x_1,y_1)=(CL_{min}(N),CL_{max}(S))$, $(x_2,y_2)=(CL_{max}(N),0)$ and $(x_e,y_e)=(N_{dep},S_{dep})$ one obtains the point $(x_0,y_0)=(N_0,S_0)$ (*Z2* in Figure 7.3). The final difficulty in computing the $Ex(N_{dep},S_{dep})$ is to determine into which of the regions (Region 0 through Region 4 in Figure 7.3) 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*:

```
      subroutine  exceed  (CLmaxS,CLminN,CLmaxN,depN,depS,ExN,ExS,ireg)
!
!     Returns the exceedances ExN and ExS (Ex=ExN+ExS) for N and S
!     depositions depN and depS and the critical load function given by
!     CLmaxS, CLminN and CLmaxN.
!     The 'region' in which (depN,depS) lies, is returned in ireg.
!
      integer(4)         ireg
      real(4)            CLmaxS, CLminN, CLmaxN, depN, depS, ExN, ExS
!
      ExN = -1.
      ExS = -1.
      if (CLmaxS < 0. .or. CLminN < 0. .or. CLmaxN < 0.) return ! error
      d1 = CLmaxN-CLminN
      dnn = depN-CLminN
      dxn = depN-CLmaxN
      dxs = depS-CLmaxS
      if (depS <= CLmaxS .and. depN <= CLmaxN .and.
     &    CLmaxS*dxn <= -d1*depS) then ! non-exceedance
        ireg = 0
        ExN = 0.
        ExS = 0.
      else if (depN <= CLminN) then
        ireg = 4
        ExN = 0.
        ExS = dxs
      else if (dxn*d1 >= depS*CLmaxS) then
        ireg = 1
        ExN = dxn
        ExS = depS
```

```
else if (CLmaxS*dxs >= d1*dnn) then
  ireg = 3
  ExN = dnn
  ExS = dxs
else
  ireg = 2
  d2 = -CLmaxS
  dd = d1*d1+d2*d2
  s = depN*d1+depS*d2
  v = -CLmaxS*CLmaxN
  x0 = (d1*s+d2*v)/dd
  y0 = (d2*s-d1*v)/dd
  ExN = depN-x0
  ExS = depS-y0
end if
                                    return
end subroutine exceed
```

For a given critical load function an exceedance can be defined for every pair of depositions (N_{dep},S_{dep}) as outlined above. Connecting points in the (N_{dep},S_{dep}) plane which have identical values of the exceedance function, results in ***exceedance isolines*** as illustrated Figure 7.4. The 'kinks' in the isolines when passing from one exceedance region to a neighbouring one can be clearly discerned.

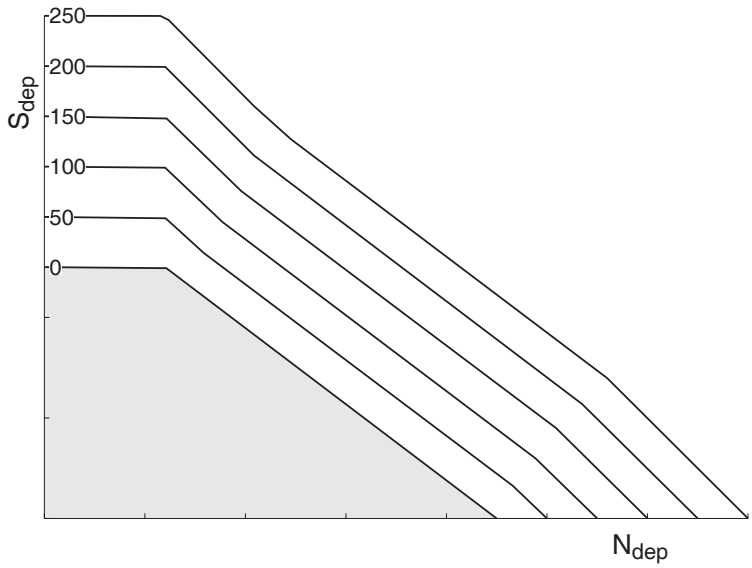


Figure 7.4: Exceedance isolines for a given critical load function. The line labelled "0" corresponds to the critical load function and delimits the grey-shaded area of zero exceedance.

7.4 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 5.4.

7.4.1 The SSWC model

In the SSWC model sulphate is assumed to be a mobile anion (i.e. leaching equals deposition), whereas nitrogen 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):

(7.11)

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

where $CL(A)$ is the critical load of acidity as computed with eq. 5.50. 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. Only in the FAB model (see below) are nitrogen processes modelled explicitly, and thus only that model 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 $S^*_{dep} + N_{le}$.

7.4.2 The empirical diatom model

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

(7.12)

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

where f_N is the fraction of the nitrogen deposition contributing to acidification (see eq. 5.66).

7.4.3 The FAB model

Since in the FAB model a critical load function for surface waters is derived from the in the same way as in the SMB model for soils, the same considerations hold as given in Section 7.2. 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 for the soil critical load function (see also Henriksen and Posch 2001).

7.5 Target Loads

In the previous sections the excess of depositions over critical loads has been defined as exceedance. In the case of target loads or target load functions the same quantities as defined above can be calculated, but if they are positive, we talk about the ***non-achievement*** of the target load; if it is zero or negative, we say the target (load) for a given year has been achieved.

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