ENVIRONMENTAL RESEARCH OF THE
FEDERAL MINISTRY OF THE ENVIRONMENT,
NATURE CONSERVATION AND NUCLEAR SAFETY

Research Report 298 22 244
UBA-FB 000204/e

Texte
80
01
ISSN
0722-186X

Trend methods for the assessment of effectiveness of reduction measures in the water system

von

PD Dr. habil. Steffen Uhlig
Prof. Dr. Peter Kuhbier

Institut für Statistik und Ökonometrie
Freie Universität Berlin

On behalf of the Federal Environmental Agency

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Publisher: Federal Environmental Agency (Umweltbundesamt)
Postfach 33 00 22
14191 Berlin
Tel.: +49/30/8903-0
Telex: 183 756
Telefax: +49/30/8903 2285
Internet: http://www.umweltbundesamt.de

Edited by: Section II 3.2
Dr. Heike Herata

Berlin, November 2001

1.(Report No.)	2.	3.

Report title: Trend methods for the assessment of effectiveness of reduction measures in the water system.

5. Authors: Uhlig, Steffen Kuhbier, Peter	8. Report date: 30.04.2000
	9. Publication date: 21.05.2001
	10. UFOPLAN Ref.No: 298 22 244
6. Performing Organisation: Institut für Statistik und Ökonometrie Freie Universität Berlin Garystr. 21 14195 Berlin	11. No of Pages: 79 (plus 105 in the annexes)
	12. No of References: 19
7. Sponsoring Agency Umweltbundesamt, Bismarckplatz 1, 14191 Berlin	13. No of Tables, Diagrams: 22 (plus 57 in the annexes)
	14. No of Figures: 45 in the annexes
15. Supplementary Notes	

16. Abstract:

Riverine inputs are highly depending substance-specifically on flow rate and other climatic factors. In order to prevent that climatic influences deteriorate the trend detectability, an appropriate adjustment of the measurement data is necessary. Subject of the research project is therefore a concept for the adjustment and trend analysis of these input data.

The basic concept for adjustment and trend analysis of riverine inputs is as follows: After providing monthly or biweekly data, monthly or biweekly adjusted loads are calculated with an adjustment procedure based on a dynamically specified concentration-flow function. Then the annual adjusted load is obtained by averaging the monthly or biweekly adjusted data. In the next step a trend analysis of the annual adjusted load is performed, using the LOESS smoother or the test of Mann-Kendall. Finally a power analysis is performed in order to assess the trend sensitivity of the method.

Nine adjustment methods were tested at seven parameters (NO_3-N, NH_4-N, P_{total}, PO_4-P, Cd, Pb and suspended matter) measured biweekly in the Rhine River (Lobith) and monthly in the Ems River (Herbrum). For the Rhine River, the use of adjusted loads instead of the OSPAR load increases trend detectability considerably for nitrate, total P and suspended matter, whereas for the other substances only small differences can be observed. Using concentration mean values reduces the power substantially. For the Ems River the use of adjusted loads or concentration mean values instead of the OSPAR load increases trend detectability for all nutrients.

The investigations confirm that in general all adjustment methods are applicable, but there is no method which is optimal for every river and every substance. For the adjustment of nutrient loads a method based on a local regression model with reciprocal flow rate allows considerable improvement of the trend sensitivity and seems to therefore to be reasonable. For heavy metals only small advantages by adjusted load could be observed, although this might be due to chemical-analytical problems.

17. Keywords: Load; Adjustment; Trend; Monitoring; Statistical Test

18. Price	19.	20.

1.(Berichtsnummer)	2.	3.
Titel des Berichts: Methoden der Trendabschätzung zur Überprüfung von Reduktionszielen im Gewässerschutz		

5. Autoren: Uhlig, Steffen Kuhbier, Peter	8.Abschlussdatum: 30.04.2000
	9. Veröffentlichungsdatum: 21.05.2001
	10. UFOPLAN-Nr.: 298 22 244
6. Durchführende Institution: Institut für Statistik und Ökonometrie Freie Universität Berlin Garystr. 21 14195 Berlin	11. Seitenzahl: 79 (zuzüglich 105 Seiten im Anhang)
	12. Literaturangaben: 19
7. Fördernde Institution: Umweltbundesamt, Bismarckplatz 1, 14191 Berlin	13. Tabellen und Diagramme: 22 (zuzüglich 57 Tabellen und Diagramme im Anhang)
	14. Abbildungen: 49 Abbildungen im Anhang
15. Zusätzliche Angaben	

16. Kurzfassung:

Flussfrachten sind in hohem Maße - je nach Substanz – von der Durchflussrate und anderen klimatischen Faktoren abhängig, und um zu verhindern, dass klimatische Einflüsse die Nachweisbarkeit von zeitlichen Trends in diesen Eintragsdaten verschlechtern, ist eine Adjustierung der Messdaten erforderlich. Gegenstand des Vorhabens ist daher ein Konzept für die Adjustierung und Trendanalyse dieser Eintragsdaten.

Das Konzept ist wie folgt strukturiert: Auf der Basis monatlicher oder vierzehntägiger Messdaten werden monatliche bzw. vierzehntägige adjustierte Frachten unter Verwendung einer dynamisch angepassten Konzentrations-Durchfluss-Funktion berechnet. Die adjustierte Jahresfracht ergibt sich dann mittels Durchschnittsbildung aus den monatlichen bzw. vierzehntägigen adjustierten Frachten. Auf Basis dieser Jahreswerte wird schließlich unter Verwendung des LOESS-Trendschätzverfahrens eine Trendanalyse durchgeführt. Abschließend wird im Rahmen einer Power-Analyse die Trendsensitivität des Verfahrens überprüft.

Neun Adjustierungsmethoden wurden an sieben Parametern (NO_3-N, NH_4-N, P_{total}, PO_4-P, Cd, Pb und Schwebstoffkonzentration) getestet, die vierzehntägig im Rhein bei Lobith und monatlich in der Ems bei Herbrum bestimmt wurden. Für den Rhein ermöglicht die Verwendung adjustierter

Frachten anstelle nicht-adjustierter Werte eine erhebliche Verbesserung der Trendsensitivität bei NO_3-N, P_{total} und Schwebstoffgehalt, während bei den anderen Parametern nur kleine Unterschiede festgestellt werden konnten. Hingegen führt die Verwendung von jährlichen Konzentrationsmittelwerten zu einer Verringerung der Trendsensitivität. Für die Ems ermöglichen adjustierte Frachten und jährliche Konzentrationsmittelwerte gegenüber nichtadjustierte Frachten für alle Nährstoffe eine höhere Trendsensitivität. Generell bestätigen die durchgeführten Auswertungen die Praktikabilität der hier entwickelten Adjustierungskonzeption, wobei jedoch keine Methode für alle Flüsse und Substanzen als optimal erscheint. Zur Adjustierung von Nährstoffen erscheint eine auf einem lokalen Regressionsmodell mit reziproker Durchflussrate basierende Methode zweckmäßig und ermöglicht im Vergleich zur OSPAR-Fracht eine wesentliche Verbesserung der Trendsensitivität. Bei den untersuchten Schwermetallen werden geringere Vorteile ermittelt, wobei jedoch zu vermuten ist, dass dies zumindest zum Teil durch chemisch-analytische Probleme verursacht wird.
17. Schlagwörter: Fracht; Adjustierung; Trend; Monitoring; Statistischer Test

18. Preis	19.	20.

Contents

List of Illustrations

List of Quantities

α	Model parameter for the effect of the reciprocal runoff on the concentration or the constant part of the LQ function
α_i	Model parameter for the constant part of the LQ function in year *i*
$\hat{\alpha}_i$	Estimated value for α_I
α_j	Model parameter for the constant part of the LQ function in season *j*
α_{ij}	Model parameter for the constant part of the LQ function in year *i* and season *j*
β	Model parameter for the constant part of the CQ function or for the flow-dependent part of the linear LQ function
$\hat{\beta}$	Estimated value for β
β_i	Model parameter for flow-dependent part of the linear LQ function for year *i*
$\hat{\beta}_i$	Estimated value for β_i
β_{ij}	Model parameter for flow-dependent part of the linear LQ function for year *i* and season *j*
δ	Model parameter for linear temporal trend
$\varepsilon_t = \varepsilon_{ij}$	Error term
ε	Vector of error terms
γ	Model parameter for the effect of the reciprocal lagged runoff
$\gamma_1, \gamma_2, \gamma_3, \gamma_4$	Model parameter for the season component
γ_{ij}	Model parameter for the exponential LQ function
λ	Model parameter for the non-linear part of the CQ function
λ_1, λ_2	Control parameter for method N
λ_{ij}	Adjustment factor

η	Model parameter for the temperature effect
ρ	Serial correlation of annual runoff
σ	Standard deviation
σ^2	Variance
σ_{rel}	Relative standard deviation
AIC	AIC criterion for the evaluation of the model fit
ALPHA	Error probability for the trend test
B(Q)	CQ function in vector form
C	Vector of concentration measurements
$c(q)=c_{ij}(q_{ij})$	CQ function
$c_{ij} = c_t$	Concentration measured (mg/l for nutrients, µg/l for heavy metals) at time $t=t_{ij}$
c_{ij}^*	Concentration due to point sources
c_{ij}^+	Concentration due to diffuse sources
Cov	Covariance operator
d	Model parameter for a non-linear LQ function
df	Number of degrees of freedom
E[]	Expectation operator
$f(q;s) = f_i(q,s)$	Model curve in the TRANSPOS model, depending on runoff q, season s and period i
$F_{T_{n-df},\delta}$	Distribution function of the non-central t distribution
i	Index of the year. In the TRANSPOS model: Index of the period
j	Sample index within the year (season index)
k_i	Coefficient in the TRANSPOS model
k_i^*	Coefficient in the extended TRANSPOS model

L	Load
L_a	Vector of adjusted annual loads
L_i	Load value in the year *i* (t/a for nutrients, kg/a for heavy metals)
$L_{i,a}$	Adjusted load in the year *i* (t/a for nutrients, kg/a for heavy metals)
$L_{i,est}$	Mean load in year *i*
$L_{i,mean}$	Estimated load in year *i*
$L_{i,a}^{*}$	Load due to point sources in year *i*
$L_{i,a}^{+}$	Load due to diffuse sources in year *i*
$L_{i,OSPAR}$	OSPAR load in the year *i* (t/a for nutrients, kg/a for heavy metals)
L_{ij}	Load (transport) at time t_{ij} (g/s for nutrients, mg/s for heavy metals)
$L_{ij,a}$	Adjusted load at time t_{ij} (g/s for nutrients, mg/s for heavy metals)
$L_{ij,e}$	Estimated load at time t_{ij} (g/s for nutrients, mg/s for heavy metals)
$L_{ij,m}$	Mean load at time t_{ij} (g/s for nutrients, mg/s for heavy metals)
m	Duration of a year expressed in units of sampling times
M	Number of periods (measurements) in the year
MQ	Long-term mean runoff (m^3/s)
N=n	Sample size
Q	Runoff (m^3/s)
$q_{0ij} = q_{0j} = q_{0t}$	Long-term monthly mean of runoff at time $t=t_{ij}$ (m^3/s).
$q_{ij} = q_t$	Runoff (m3/s) at the t_{ij} point of time
q_{t-1}	Runoff (m^3/s) at day *t*-1
q_{ij-1}	Runoff (m^3/s) at time $t=t_{i,j-1}$
$\overline{q^2}$	Mean of squared runoff
$\overline{q}_i$	Mean runoff in year *i* (m^3/s)

p	Model parameter for the effect of the runoff in the simulation model
rho	Serial correlation coefficient
RSS	Square sum of residuals
s	Season in TRANSPOS model
$s(q)=s(q_t)$	Spline function
$s(q_{0t})$	Spline function for $q=q_{0t}$
S(Q)	Vector form of concentration-independent part of the additive adjusted loads
$s_i(q_{ij})$	Spline function in year *i*
$S(\alpha,\beta)$	Estimation functional for method N
Season	Season component of CQ function
SIGMA	Control parameter for Hebbel's model
S_{Ratio}	Quotient of standard deviation of the adjusted loads and the standard deviation of the OSPAR load
s_{RES}	Residual standard deviation
s_t	Seasonal component in Hebbel's model
t	Sampling time
T	Within the adjustment step: Number of years. Within the calculation of the power: Test statistic for the trend test.
$t_1,\ldots,t_n$	Sampling times
t_{ij}	Time of sampling for the *j*th sample in the *i*th year
$t_{n\text{-}df,1-\alpha}$	Quantile of the t distribution with *n-df* degrees of freedom
u_t	Trend component in Hebbel's model
u_i	Random variable in the simulation model
v_{ij}	Random variable in the simulation model

W	Smoother matrix
w_{ij}	Random variable in the simulation model
w_t	Water temperature at time *t*
x	Within the trend analysis: Index of the year. Within Hebbel's model: vector of reciprocal flow data
y	Annual value (load or concentration)
y_i	Annual value in year *i*
z	Vector of flow-corrected concentrations in Hebbel's model
$\hat{z}$	Estimation vector for *z*
z_t	Flow-corrected concentration in Hebbel's model

List of Abbreviations

4.INK	Fourth International Conference on the Protection of the North Sea
A0	Standardisation of the OSPAR load to the long-term mean runoff (Section 5.2.2)
BC	Extension of the TRANSPOS method (Section 5.17.1)
Cd	Cadmium
CQ function	Concentration runoff function
CSV	File format compatible to EXCEL
H	Hebbel's method (Section 5.3)
HARP-NUT	OSPAR-Guidelines for Harmonised Quantification and Reporting Procedures for Nutrients
HELCOM	Helsinki Commission
ICES	International Council for the Exploration of the Sea
ICES-ACME	ICES Advisory Committee of Marine Environment
ICES-WGSAEM	ICES Working Group on Statistical Aspects of Environmental Monitoring
ID	Identification number
ICPR	International Commission for the Protection of the Rhine
INPUT	Working Group on Inputs to the Marine Environment
L1	Local regression with season (Section 5.4)
L2	Local regression with season and lagged runoff effect (Section 5.5)
L3	Local regression with temperature and lagged runoff effect (Section 5.6)
L4	Local regression with season temperature & lagged runoff effect (Section 5.7)
L5	Local regression with a non-linear component in the LQ function
LOESS	Cleveland's smoother
LQ function	Load runoff function
N	Non-parametric smoother as per Stalnacke (Section 5.2)
NH_4-N	Ammonium
NO_3-N	Nitrate
OSPAR	Oslo Paris Commission
OSPAR load	Annual load according to the OSPAR formula
OSPAR-INPUT	OSPAR Working Group on Inputs to the Marine Environment
Pb	Lead
PO_4-P	Ortho-Phosphate

P_{Total}	Phosphorus
S1	Estimation using splines (Section 5.8)
S2	Estimation using local splines (Section 5.9)
TRANSPOS	Brunswig's load calculation method
UBA	Federal environment agency
VBV	„Generalized Berlin Method", a statistical trend analysis method developed by Heiler and Hebbel
WMF	Windows-Meta-File
Y1	Direct method for the calculation of annual adjusted loads applying a linear LQ function
Y2	Direct method for the calculation of annual adjusted loads applying a non-linear LQ function

1 Introduction

1.1 Objective

The project aims to develop a method for the quantitative assessment of a statistically validated trend for waterborne inputs into the North and Baltic Seas. With this trend assessment method it should be possible to ascertain whether the measures undertaken in the catchment area for reducing material inputs at the source also result in an improvement in the water quality as well as in a reduction in the inputs into the North and Baltic seas.

In accordance with international agreements (such as OSPAR HELCOM, 4 INK, ICPR) Germany is committed to reduce the inputs of primary substances into water bodies. Thus it was decided in the course of the Second International Conference for the Protection of the North Sea in 1987 that measures be taken to reduce the inputs of nutrients and persistent toxic substances, with a 50% reduction being targeted for the period between 1985 and 1995. For substances for which this target has not been met, it was decided at the Fourth Conference for the Protection of the North Sea that the reduction target be retained until 2000.

There is as yet no quantitative evidence that measures adopted in the catchment area (reductions at the sources) have also brought about a reduction of input via the rivers into the maritime area. This problem should be solved both in the OSPAR and Helsinki Commissions as part of the mandate of the "Working Group on Inputs to the Marine Environment (INPUT)". However for this, the development of a statistically well-founded method of trend assessment for riverine inputs is mandatory. Trend assessment for monitoring reduction targets through riverine loads pose problems since loads constitute values calculated from concentration and runoff data. Thus while determining the reduction rates for riverine loads, fluctuations in river runoff alone could effect an increase in loads in two selected years, despite reduction measures having been implemented in the river catchment area. This may be explained by the fact that during years of heavy precipitation with heavy runoff, the inputs to the maritime area tend to be higher than in dry years with low runoff. For this reason it is not just the loads alone which should be taken into account while evolving such a trend assessment method but, more importantly, the runoff, concentration and temperature.

With the help of a statistically backed trend assessment method it could be possible to undertake a uniform assessment of the riverine input data collected over several years within the framework provided by the OSPAR Commission, the Helsinki Commission as well as the River Basin Commissions. This would also put Germany in a position to examine whether the measures already introduced to meet international reduction targets are adequate or whether additional measures are necessary in the catchment area in order to effectively reduce inputs into the maritime areas.

A joint workshop organized by OSPAR-INPUT and ICES-WGSAEM (ICES: International Council for the Exploration of the Sea; WGSAEM : Working Group on Statistical Aspects of Environmental Monitoring) was held in Copenhagen in March 1997 with the aim of developing a method for the quantitative assessment of a statistically based trend for riverine inputs into the North and Bactic Seas. Subsequently the Netherlands was entrusted with the task of working on the further development of a statistical method on the basis of the results of this workshop. The fruits of these efforts are for the most part contained in a software programme ("Trend-y-tector") for analysing annual data. This programme was introduced in OSPAR-INPUT in 1998. Following this, OSPAR-INPUT decided that further investigations were necessary particularly with regard to :

- the inclusion of appropriate adjustment methods for compensating the effects of climate variability (such as runoff, temperature, precipitation)
- the inclusion of a power function as well as
- the consideration of monthly data

Thereafter OSPAR decided in 1998 to entrust ICES with the further investigation of statistical methods. However, since there is as yet no scientific method available for adjusting the monthly and annual measurement data in order to compensate the effects of climate variability, the R&D project presented here was initiated by the Federal Environment Agency (Umweltbundesamt) with the aim of developing a statistical concept that enables

- The adjustment of riverine loads, determined on the basis of the OSPAR river measurement sites, with regard to temperature, suspended matter, runoff etc.
- The determination of temporal trends for these parameters on a weekly, monthly and yearly basis with the help of robust, varying and non-parametric methods.
- The assessment of the quality of the data on the basis of the power function.

This concept shall directly draw upon the results in the ICES as well as on these discussed in the joint ICES/OSPAR workshop (Copenhagen 1997) and in OSPAR-INPUT (Schwerin 1998). Furthermore, it is proposed that a data and programme structure be drawn up for a software which will make it possible to retrieve the newly developed statistical protocols for routine purposes as well. The structure proposed to be implemented here shall be flexible and modular so as to enable the software to be easily changed and expanded in relation to the results of research. The development of the software, that is first of all the definition of the data structure and the basic functions and menus, shall proceed ride by side with the development of the method.

1.2. Project planning and procedure

Close cooperation was sought, both at the national and international levels, in order to ensure a broad-based acceptance of the results. Adjustment concepts as well as concrete recommendations for fixing adjustment parameters were discussed with the Federal Länder (states) during project meetings. Cooperation at the international level was ensured by the participation of one of the two project leaders in the ICES-WGSAEM and the ICES-ACME (Advisory Committee of Marine Environment) as well as through the discussion of the results in the INPUT working group.

1.2.1 Project Discussion with the Federal Länder

On 4th June 1998 an initial discussion for arriving at a joint consensus on the components of the R&D project was conducted with the concerned Federal Länder in the UBA (Federal Environment Agency). The following approaches were introduced and deliberated on in the course of this discussion :

- The recommentation made by the Netherlands to OSPAR-INPUT for a trend analysis of non-adjusted annual loads using the so-called trend-y-tector.
- A loglinear regression model developed by Bjerkeng, Norway, that takes into consideration lagged runoff.
- The VBV (Generalized Berlin Method) developed by Heiler and Hebbel for economic time series.
- The Kiel Method for load calculation developed by Brunswig using a CQ function constituted on the basis of measured concentration and related runoff.
- The window method developed by Behrendt in which the loads are divided into three runoff areas. These three runoff areas can then be individually subjected to a trend analysis. Here it may be pointed out that the low-water area reflects the flow of loads primarily caused by point sources.

As opposed to this, the flow of loads in the high-water area is for the most part determined by diffuse sources. It was generally agreed that an adjustment using a suitable CQ function is necessary for determining a statistically corroborated trend. The adjusted data sets should than be subjected to a statistical trend analysis where a statistical approach shall be selected whereby a monotonic trend can be demonstrated. On October 1st 1998 the second project discussion was held in the Federal Environment Agency (UBA). At this discussion a conceptional recommendation for approaching the trend assessment of load was put forth by the researcher along with the initial test results on the various approaches for the adjustment and trend analysis of loads.

The participants of the meeting agreed that the adjustment should be carried out with the help of raw data and that the annual load which is then calculated on the basis of the adjusted data will be subjected to a trend analysis (see Fig. 3.1). There was also general consensus that a comparative analysis of the following methods of adjustment in particular be performed:

- Modelling of the CQ function according to Brunswig's approach.
- Taking into account lagged runoff in accordance with Bjerkeng's approach, with however an additive and not a loglinear parametrisation of the CQ function having to be used.
- The VBV method with exogenous factors of influence.
- The method developed by P. Stalnacke for adjusting nutrient loads, based on non-parametric smoothing.
- Inclusion of temperature as a substitute for seasonal effect.
- Calculation of the annual load taking into account the long-term mean runoff.

During the third and fourth meetings held on 3rd March 1999 and 30th June 1999 respectively, the abovementioned methods were discussed in the light of the test results for the measurement sites of Lobith (Rhine) and Hebrum (Ems) for the parameters NO_3-N, P_{total}, PO_4-P , Cd, Pb and suspended matter.

Additionally, an alternative method shall be tested whereby trend analysis and adjustment will not be undertaken separately one after the other but as part of a combined process.

More far-reaching evaluations for the said parameters as well as for the NH_4-N load were discussed at the 5th meeting on October 14th 1999 inter alia for trend analysis and the power function as well as for the number of measurement years required so as to render a particular method deployable.

Finally, at the last meeting on February 24th 2000 the subject of discussion involved Brunswig's Kiel Method as well as a final evaluation of the method developed. It was found that none of the methods investigated were equally "optimal" for all the parameters concerned but that each of these methods had its specific advantages and disadvantages. Consequently it was not possible to arrive at a final assessment or evaluation during the session.

1.2.2. Discussions in ICES-WGSAEM and OSPAR-INPUT

Diverse adjustment methods were intensely discussed during the WGSAEM discussions of March 1999 and March 2000. Both the discussions and the results of these meetings have been documented in detail in the annual reports of these working groups. These reports have again been discussed by ICES-ACME and the most important results published in its annual reports for 1999 and 2000 in revised form.

The focus of the work undertaken by WGSAEM 1999 involved the question as to how adjusted loads could be interpreted, while WGSAEM 2000 mainly concentrated on the investigation of statistical properties. The researcher also participated in the OSPAR-INPUT 1998 meetings in Schwerin and London where demands to be met by trend analysis were discussed along with the basic approach.

2 Load Calculation According to OSPAR-INPUT

In order to determine the annual load in accordance with the calculation rule set down by OSPAR-INPUT, both the concentration and runoff values measured at regular intervals as well as the average runoff are required.

If c_{ij} denotes the measured concentration of the *j*th sample, *j=1,.....*m, in year *i* and q_{ij} denotes the corresponding runoff value, then the riverine load as per OSPAR-INPUT for the year *i* may be expressed as follows :

$$L_{OSPAR,i} = 31{,}5576 \frac{\bar{q}_i}{\sum_{j=1}^{m} q_{ij}} \sum_{j=1}^{m} c_{ij} q_{ij}$$

with the average runoff being $\bar{q}_i$ in the year *i* (m^3/s). The unit of the annual load measured thus corresponds with

- t/a, if the unit of measurement used for the concentrations is mg/l
- kg/a, if the unit of measurement used for the concentrations is µg/l

The factor 31,5576 may be computed as:

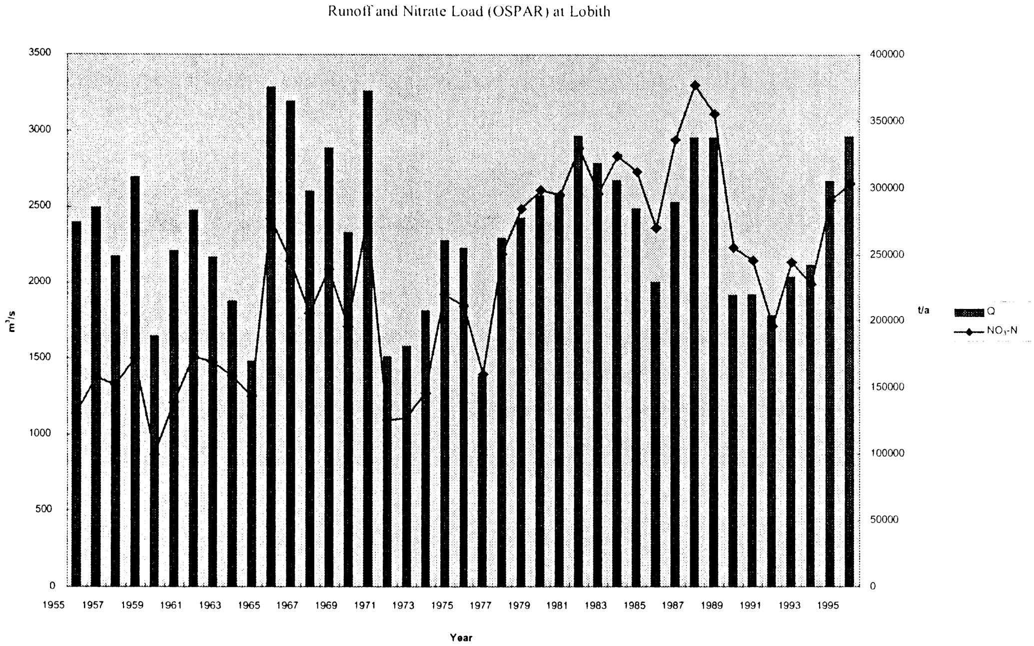
$$\left[\frac{t}{a}\right] = 10^9 \left[\frac{mg}{a}\right] = \frac{10^9}{365{,}25 \cdot 24 \cdot 3600}\left[\frac{mg}{s}\right] = \frac{10^9}{31{,}5576 \cdot 10^6}\left[\frac{mg}{l} \cdot \frac{l}{s}\right] = \frac{1}{31{,}5576}\left[\frac{mg}{l}\right]\left[\frac{m^3}{s}\right].$$

Therefore the OSPAR load can be interpreted as a quantity which is based on a flow-corrected arithmetic mean of the measured transport $c_{ij}q_{ij}$ and which is converted to an annual index. In the following text the load refers either to the annual load (in units of t/a or kg/a) or to the transport (in units g/s or mg/s).

Depending on the substance involved, riverine loads are subject to more or less strong climatic influences such as precipitation, runoff and temperature. The OSPAR loads' dependence on runoff, particularly for nitrate (NO_3-N) measured at Lobith/Rhine, is conspicuous. Fig. 2.1 shows the annual mean runoff q_i and the corresponding OSPAR-loads $L_{OSPAR,i}$ for the period 1955-1995. It may be noted here that a similarly highly conspicuous form of runoff dependence results even with other load-calculation formulas and particularly without the weighting of average runoff $\bar{q}_i$.

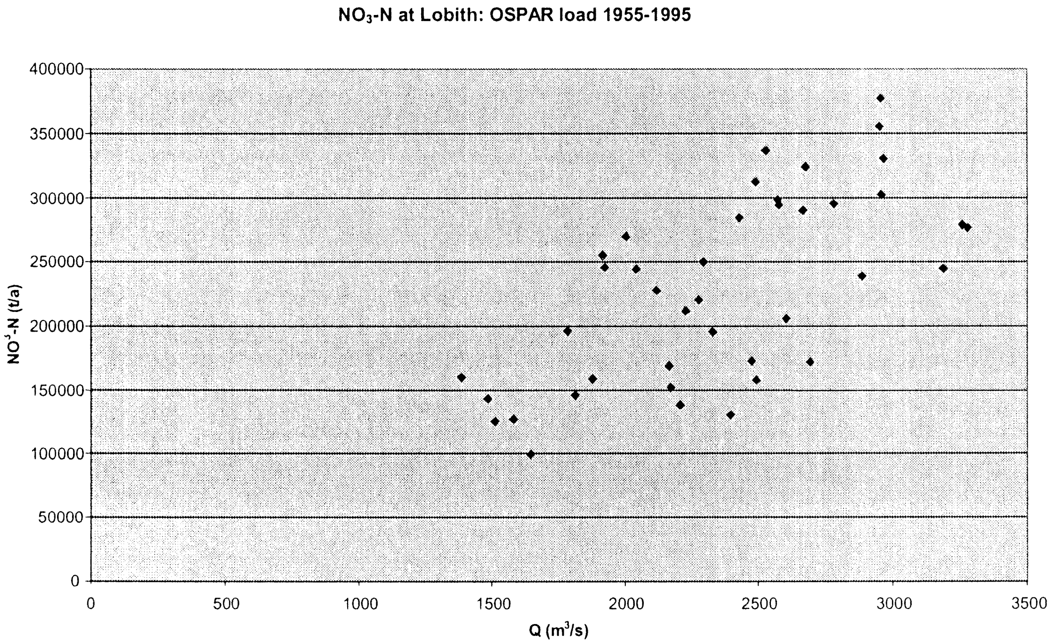
The correlation between runoff and load is even more evident in the scatter diagram shown in Figure 2.2. Despite considerable temporal variations in the annual load there is an almost proportional relationship that comes to light.

Figure 2.1



This goes to say that the investigation of anthropogenically induced changes in the loads as a result of marked fluctuations in the mean annual runoff is rendered much more difficult.

Figure 2.2


NO3-N at Lobith: OSPAR load 1955-1995
400000
350000
300000
250000
200000
150000
100000
50000
0
NO3-N (t/a)
0
500
1000
1500
2000
2500
3000
3500
Q (m3/s)

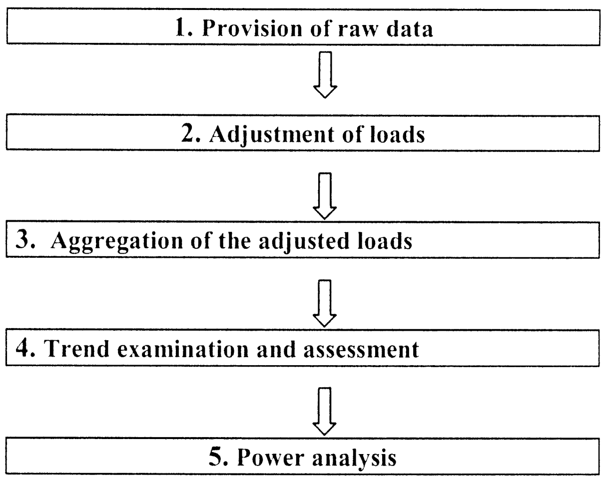
3 Concept for Load Adjustment and Trend Analysis

In order to prevent the detectability of temporal trends in annual loads getting worse as a result of fluctuations in the runoff quantity, an adjustment converting the input data into a "mean" (long-term) runoff level is indispensable. It may be noted here that not only is trend sensitivity adversely affected but that meteorological cycles may also cause fluctuations in the runoff quantity which in turn induces artificial trends in the load values, these being even observable where no anthropogenic trends exist. Therefore especially with short series, one has to reckon with statistical trend tests exceeding the given significance level in a manner that is inadmissible.

Adjustment takes place on the basis of raw data in accordance with the decision taken by OSPAR-INPUT, 1999 (Fig.3.1). The adjusted loads shall then be compiled into annual loads before trend analysis is undertaken on the basis of the adjusted annual loads. Finally the trend sensitivity of the method shall be examined within the scope of a power analysis, Examining for trend sensitivity is particularly significant where no trend could be ascertained.

Fig. 3.1

Conceptual Approach for Adjustment and Trend Analysis



In keeping with the conceptual approach described in Fig. 3.1, temporal trends are not recorded on the basis of individual measurement values but on the basis of annual values. The use of annual values rather than individual values has the disadvantage of a theoretically lower level of efficiency (power) for estimating and identifying a trend. This is balanced out by the advantage of simpler handling and a simpler statistical method. It may be noted that an automatic process is necessary in view of the large number of data sets to be evaluated, so much so that an individual adjustment of a complex time-series analytical model does not appear feasible for trend analysis while examining sets of measurements recorded on a monthly or fortnightly basis, a consideration of autocorrelation proves to be absolutely essential, thereby rendering a complex individual time-series analysis indispensable. On the other hand it appears that for annual values, autocorrelation in first approximation may even be ignored, so that the method for trend analysis becomes far simpler and allows itself to be more easily standardized.

The method outlined in Figure 3.1 has a further advantage in that the trend analytical method adopted for non-adjusted annual loads (OSPAR-INPUT 2000) can also be used for adjusted loads without any modification. This ensures that the adjustment is accepted without once again being called into question because the trend analytical method adopted earlier had to be modified or another method deployed depending on the load series. A sound comparability of results is assured because the very same trend calculation method can be used both for adjusted loads as well as for non-adjusted load series which had been determined on the basis of a single measurement per year.

4 Provision of Raw Data

Within the framework of the concept used here, the calculation of loads requires a set of measurements of concentrations measured at regular intervals either monthly or more frequently. It is recommended that standard units of measurement be used such as mg/l for nutrients and µg/l for heavy metals. Firstly, all the concentration measurements falling below the limit of detection or determination shall be replaced with appropriate substitute values in preparation for adjustment and trend analysis. A frequently accepted approach involves putting down 50% of the concerned limit of detection or determination for this purpose. It should however be borne in mind that this approach can create artificial trends if in course of time the limits of detection and determination get reduced as a result of analytical advances.

Further, for every measurement value, the corresponding runoff value expressed in the unit of measurement m^3/s is required together with the date of sampling. Also required is the long-term monthly mean runoff, likewise expressed in the unit m^3/s. In cases where the monthly mean values are not directly available these should be determined from the long-term daily runoff, with a time span of 15-30 years being recommended.

Depending on the method of adjustment used, other data will also be required. Thus the adjustment methods – based on local regression with lagged runoff effects – introduced in Sections 5.5-5.7 of the following chapter additionally require the runoff values for the days preceding the concentration measurements, while the methods presented in Section 5.6 and 5.7 also require the water temperatures in each case. Furthermore, for the method – based on non-parametric smoothing – presented in Section 5.2, precisely one measured value must be available for every month. Thus, should the measurement be available for fortnightly intervals, the mean values of the runoff and concentration values available in each case should be determined for each month.

The methods investigated in this project were examined with regard to totally 7 parameters (NO_3-N, NH_4-N, P_{total}, PO_4-P, Cd, Pb and suspended matter concentration), measured in the Rhine at Lobith and in the Ems at Hebrum. The measurements in the Rhine were carried out at fortnightly intervals while the data for the Ems was collected on a monthly basis.

5 Adjustment of the Loads

5.1 The Structure of the CQ Function

Before undertaking the actual adjustment of the loads, the question that first needs to be addressed is how the requisite CQ function (concentration – runoff function) or the corresponding LQ function (load-runoff function) is to be fixed. A monotonic correlation between runoff and load applies for many parameters as the following figures clearly show.

Figure 5.1

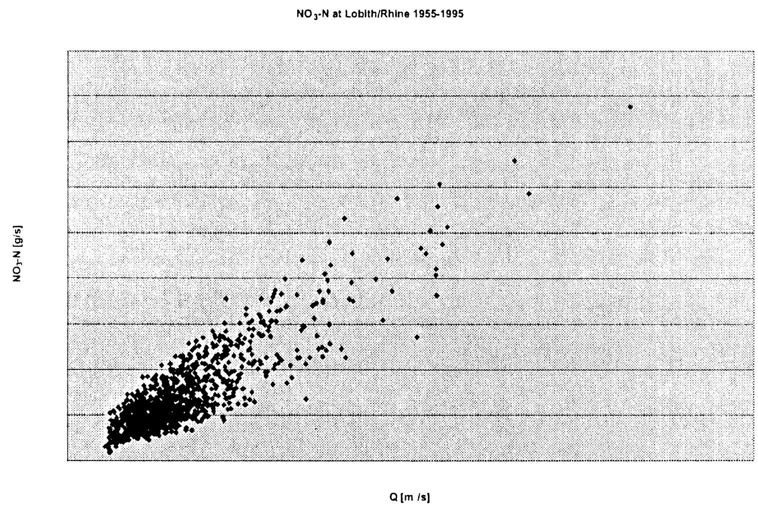


Figure 5.1 shows the load value $L_t = c_t\, q_t$ for all individual measurements carried out for NO_3-N between 1955 and 1995 at Lobith / Rhine at fortnightly intervals, for which a linear relation can obviously be established in good approximation.

Figure 5.2

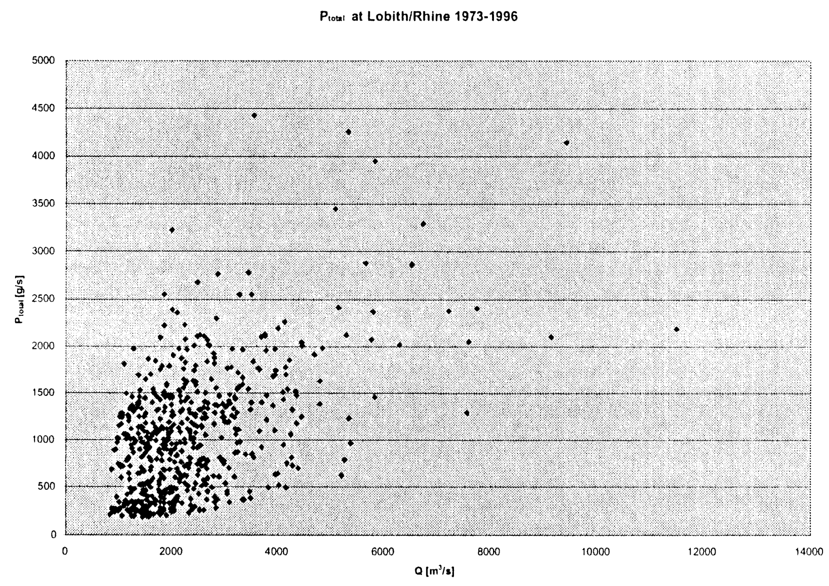


Figure 5.2 shows the corresponding results for P_{total}. In both cases a linear approximation of the relation between runoff and load is possible. However this relation is for less pronounced, and an additional difficulty for statistical analysis is the marked heteroscedasticity, that is to say the load scatter dependent on runoff. Similar representations are obtained for other rivers and other nutrient parameters while a modelling for heavy metals appears more difficult: Figures 5.3 and 5.4 show load-runoff diagrams for cadmium and load respectively.

Figure 5.3

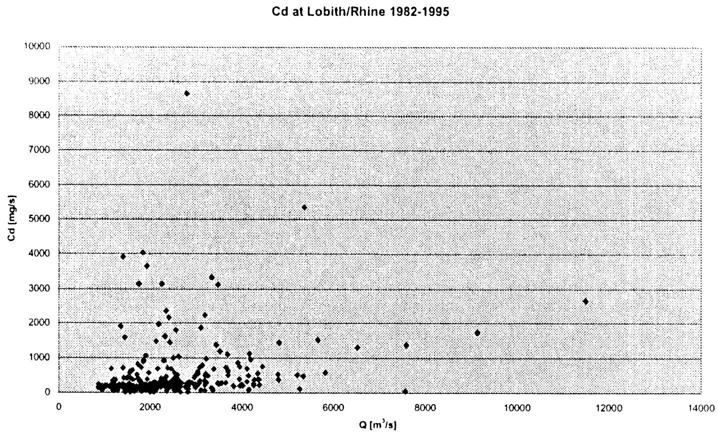
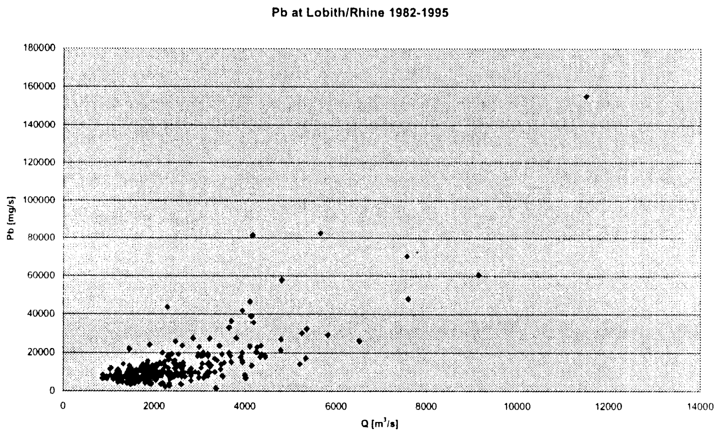


Figure 5.4



For the above two heavy metals, the relation between runoff and loads is but weak so that is may be assumed here that other influence variables play a significant role for the load of these substances.

Nevertheless in all the cases represented, there is nothing that negates the assumption that the LQ relation (load-runoff relation) is linear in its first approximation, and going hand in hand with this is the assumption that the CQ function (concentration-runoff relation) in first approximation can be described through a linear function of the reciprocal value of the runoff (1/Q). This linear relation between runoff and load constitutes the basis of the statistical methods described in Sections 5.2-5.7, these methods differing from each other with regard to the inclusion of other influence variables and in the treatment of seasonality. Non-linear relations between runoff and load are then considered in Sections 5.8 and 5.9.

5.2 Non-Parametric Smoothing as per Stalnacke (Method N)

5.2.1 Stalnacke's Recommendation

As per a recommendation put forth by Stalnacke (1996; see also the OSPAR Guidelines for Harmonised Quantification and Reporting Procedures for Nutrients – HARP-NUT – Guideline Number 7: Quantification of the Total Riverine Load of Nutrients, 2000), the load is linearly modelled as per the following equation:

$$L_{ij} = \alpha_j + \beta_{ij} q_{ij} + \varepsilon_{ij},$$

where L_{ij} = load in year i and season j

q_{ij} = runoff in year i and season j

$i = 1, \ldots, d$

$j = 1, \ldots, m$

The index i denotes the year of measurement, while j indicates the season. The Stalnacke model requires a firm time-frame, that is to say, the season index j refers to a particular month in the year. This makes it necessary to first of all appropriately arrange all the measurement values within the given frame during data processing.

However, possibilities of using this model appear limited since only the proportional parameter β and not the constant component α is dependent on index i, that is to say, this load component – which in first approximation is determined by the point sources – does indeed contain a seasonal component but is however assumed to be temporally constant over the years. This assumption appears to be not quite satisfactory, at least in cases where there is a considerable reduction in inputs from point sources, possibly giving rise to considerable distortions in the adjusted load. It is for this reason that an extended non-parametric model is being examined as part of the present investigation.

5.2.2 An Extended Non-Parametric Model

The following model is considered is as an extension of the recommendation made by Stalnacke:

$$L_{ij} = \alpha_{ij} + \beta_{ij} q_{ij} + \varepsilon_{ij} .$$

This model differs from Stalnacke's recommendation in that not only β, but even α_{ij} is dependent on the year i. The two model parameters α_{ij} and β_{ij} can be non-parametrically estimated by minimizing the following equation:

$$S(\alpha,\beta) = \sum_{i,j}(L_{ij} - \alpha_{ij} - \beta_{ij} q_{ij})^2 + \lambda_1 \sum_{i,j}(\alpha_{ij} - \frac{\alpha_{i+1,j} + \alpha_{i-1,j}}{2})^2 + \lambda_2 \sum_{i,j}(\alpha_{ij} - \frac{\alpha_{i,j+1} + \alpha_{i,j-1}}{2})^2,$$

$$+ \lambda_1 \overline{q^2} \sum_{i,j}(\beta_{ij} - \frac{\beta_{i+1,j} + \beta_{i-1,j}}{2})^2 + \lambda_2 \overline{q^2} \sum_{i,j}(\beta_{ij} - \frac{\beta_{i,j+1} + \beta_{i,j-1}}{2})^2$$

where $\overline{q^2} = \frac{1}{N} \sum_{ij} q_{ij}^2$ denotes the arithmetical mean of the squared runoff.

The penalty parameters λ_1, λ_2 must be pre-determined in an appropriate manner, thereby ensuring that with the fixing of $\lambda_1 = \lambda_2$, seasonal changes in the parameters receive the same weight as changes recorded from year to year.
In order to obtain the desired degree of adjustment of the function, the number of generalized degrees of freedom is prescribed as per Hastie and Tibshirani (1990), this number being construable as the equivalent of the number of underlying parameters.

This method based on the extended non-parametric model is called method N. The advantage of this method inherently lies in the extremely flexible modelling of the seasonal representation which permits an adequate adjustment of this representation even with extremely marked seasonal highs. Of disadvantage is the fact that the raw data has to be made available every month and that the requisite calculations are extremely time-consuming even on very advanced computers. Care should also be taken while fixing the parameters (number of degrees of freedom) in order to avoid erroneous modelling (overfitting) in the event of an unfavouable data situation (non-availability of data or such like).

5.3 Application of Hebbel's Method of Estimation (Method H)

On the basis of Hebbel's method (1992) for dividing up time series into trend, season and exogenous effects, the following model may be used for recording the concentration – runoff relation:

$$c_t = u_t + s_t + \alpha / q_t + \varepsilon_t$$

where c_t = concentration at the point of time t

L_t = load / transport at the point of time t

q_t = runoff at the point of time t

u_t = trend component

s_t = season component

α = effect of runoff on concentration (constant in time)

As opposed to the model recommended by Stalnacke, the measurement times $t_1,\dots,t_n$ during the measuring period under consideration are not necessarily equidistant.

Parameters for this model are determined on the basis of the minimization of a smoothness measurement which is defined through an appropriately fixed trend-season differential operator. Details in this regard may be obtained from the appendix as well as Section VB Glättungsverfahren of Hebbel (1997). In the case of the calculations presented here this method was used together with a linear trend with a season component of the second order. The method is dependent on a smoothing parameter SIGMA which does not explicitly find its way into the CQ relation but to the abovementioned trend-season differential operator. In the absence of other predetermined parameters it was decided to fix this smoothing parameter SIGMA in such a way that the number of generalized degrees of freedom stands at 12.

It may be noted that parameter α, which describes that portion of the load that is independent of runoff, remains constant in the model. But in order to nevertheless ensure a flexible adjustment to changed CQ relations the model is locally used, that is to say, the estimation takes place separately for every single point of time on the basis of all data within a running time window. A time window of 7 years proved to be favourable in the case of the evaluations, with the first or last seven years being considered at the beginning or end of a time series in each case, whereas in the middle region of the time series, the time window is so fixed that the point of time under investigation lies exactly in the middle of the time window. In case of non-availability of values the time window is accordingly stretched so that – in the case of monthly data – the time window encompasses exactly 7x12+1=85 individual values.

In terms of its calculation technique, Method H is extremely complicated. However it allows for a flexible adjustment of the CQ function.

5.4 Local Regression with Season (Method L1)

If the prescribed value of six degrees of freedom were to be selected for Hebbel's method described in the foregoing section, then the estimation of the adjustment parameters will be equivalent to a regression estimate on the basis of the following linear model :

$$c_t = \frac{\alpha}{q_t} + \beta + \delta t + season + \varepsilon_t,$$

with $season := \gamma_1 \sin\frac{2\pi t}{m} + \gamma_2 \cos\frac{2\pi t}{m} + \gamma_3 \sin\frac{2\pi t}{2m} + \gamma_4 \cos\frac{2\pi t}{2m}$

denoting the season component. Further m represents the length of the year, expressed in the unit of measurement used for the time t. It should be pointed out that as per this model, concentration follows a linear trend, while the effect of runoff on concentration remains constant in time. Both this model as well as Hebbel's method are appropriately used on the basis of a running time window of 7 years in keeping with the objective at hand. In case of non-availability of values, the time-window will be accordingly extended so that it encompasses exactly 7x12+1=85 individual values in terms of monthly data.

Method L1 is by its very nature closely related to Method H and generates similar results as a rule. The advantage with Method LI is that it is far less complicated in its calculations and, given an extremely simple model structure, assures an extremely robust behaviour even where the data situation is sadly inadequate.

5.5 Local Regression with Season and Lagged Runoff Effect (Method L2)

The CQ relation is more often than not dependent on not just the current runoff but also on earlier runoff. Experience has shown here that higher concentrations should be expected with increasing runoff and lower concentrations with decreasing runoff. It therefore follows that the model described in the foregoing section be extended for a lagged runoff effect as below:

$$c_t = \frac{\alpha}{q_t} + \frac{\gamma}{q_{t-1}} + \beta + \delta t + season + \varepsilon_t$$

where q_{t-1} represents the runoff measured on the previous day, and *season* is defined as in the previous section. It should be noted here that often a runoff value is available on day t-1 though there is no concentration value, for concentration measurements are typically carried out in approximation on a biweekly or monthly basis.

Due to the higher number of parameters and the consequently somewhat lower stability of the estimation values, it proved useful to extend the window during regression estimation from 7 to 8 years. This means that a higher flexibility in model adjustment is obtained at the cost of a somewhat lower temporal flexibility.

5.6 Local Regression with Temperature and Lagged Runoff Effect (Method L3)

In order to obtain a – as far as possible – simple modelling of the CQ relation, the option that seems logical is to substitute the season modelling through a temperature effect which possibly reflects a similar trend for the year. Thus the following CQ relation is obtained in amendment of the model described in Section 5.5:

$$c_t = \frac{\alpha}{q_t} + \frac{\gamma}{q_{t-1}} + \beta + \delta t + \eta w_t + \varepsilon_t$$

where w_t denotes the water temperature on day t. Both for this model as well as for Method L1, parameter estimation is based on a running time window, with the more instable behaviour of the estimation function (determined in preliminary tests) prompting the choice of a time-window extended to eight years.

5.7 Local Regression with Season, Temperature and Lagged Runoff Effect (Method L4)

If the two models described in Sections 5.5 and 5.6 are combined, then the following CQ relation is obtained:

$$c_t = \frac{\alpha}{q_t} + \frac{\gamma}{q_{t-1}} + \beta + \delta t + \eta w_t + season + \varepsilon_t$$

where w_t again denotes the water temperature on day t. The parameter estimation of this model takes place on the basis of a running time window again with a duration of eight years.

5.8 Estimation Using Splines (Method S1)

The methods described above assume that the runoff-load relation is approximately linear. In the case of parameters for which this approximation is not justified, a flexible adjustment of the CQ relation could be obtained using a cubic spline. The calculation of this cubic spline may be understood as linear smoothing, with the smoothing parameter being fixed through the degrees of freedom, that is to say, the course of the linear representation (as per Hastie and Tibshirani's approach). A value of approximately 4 is prescribed for this course. If s denotes the spline function, then the CQ relation can be expressed as:

$$c_t = s(q_t) + \varepsilon_t$$

Method S1 is based on the assumption that the spline is determined on the basis of all available measurement values, in other words what is assumed is a global, trend-free dependence between runoff and concentration. An assumption of this nature in certainly not appropriate for long series, but for short series which are not longer than 7 or 8 years, the assumption of a statistical CQ relation for load adjustment appears to be a simple and practicable method. The multiplicatively adjusted load at time t may be expressed as follows:

$$L_{.} = \frac{s(q_0\ )q_0}{s(q\ )q} L$$

In other words, apart from the relation between the current runoff q and the long-term runoff mean q the relation between the spline values at the points q and q is crucial for adjustment.

5.9 Estimation Using Local Splines (Method S2)

In order to represent temporal trends more efficiently it is recommended that the spline calculation not be carried out globally but that a window technique be used here too as with methods L1 to L4. A small data window would suffice since no further parameters are to be considered. Thus for method S2 a window with a span of three years was used for spline calculation.

5.10 Inclusion of a Non-Linear Component into the Load-Runoff Relation

The use of the parametric CQ function provides an alternative to the modelling of the CQ relation using cubic splines:

$$c(q) = \beta + \alpha/q + \lambda q^d \ ,$$

where β, α, λ and d represent the unknown model parameters to be estimated.

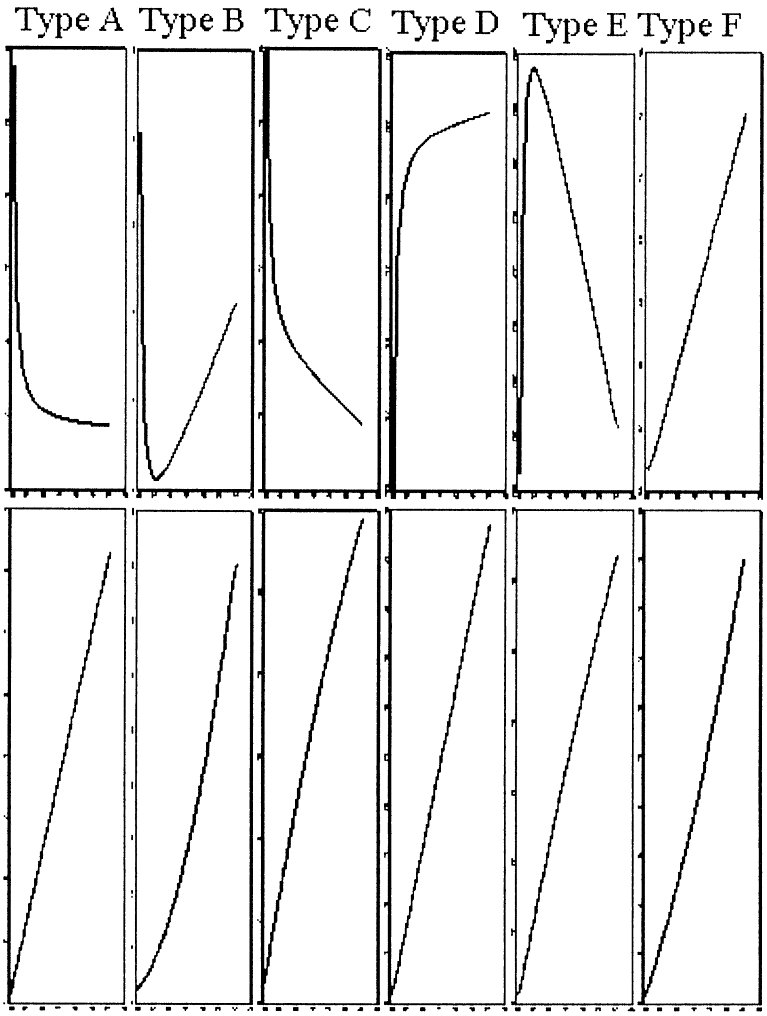
A basic prerequisite for the existence of a valid method of estimation is that the model equation pertaining to the unknown parameters is identifiable, that is to say, there should be only a single possible parameter combination for every possible line of function c(q). This prerequisite of identifiability is not assured with this model, for with d=0, the fixing of α and λ is no longer firm and clear-cut. A solution that is basically acceptable from the statistical point of view is to prescribe a lower limit for parameter d, for instance 0.5, which no value should fall below. Some methods of estimation at least are in a position to take such restrictions into account in the algorithm of estimation. On the other hand there is also the question of the interpretability of the results if the method of estimation actually yields the value of the lower limit for d. One would then have to put up with the objection that another lower limit would have yielded another value, and that the use of a specific lower limit is justified only when there are actually well-founded reasons for doing so from the hydrological point of view.

If the estimation of the parameter d has to be given up for the abovementioned reasons, then the only way out is to fix parameter d on the basis of hydrological considerations at the very start and to confine oneself to the estimation of parameters α, β and λ. It may be pointed out at this juncture that even in such a restricted type of model, there is scope for sufficiently flexible adjustments in the concentration-runoff relation. The figure 5.5 reproduced on the following page presents six concentration-runoff relations (top row) and the corresponding load-runoff relations (bottom row) which were determined on the basis of the abovementioned model for d=1 and various parameter combinations. These relations approximate the six types of a concentration-runoff or load-runoff relation described by Behrendt (1993). If one extends the model by a linear trend and a seasonal component of the second order, one devises the CQ function

$$c_t = \frac{\alpha}{q_t} + \lambda q_t + \beta + \delta t + season + \varepsilon_t$$

with season being defined as in Section 5.4. This method was tested on some parameters on a trial basis. It was found here that the result obtained only differed slightly from those yielded by Method L1. Further experiments had to be abandoned for lack of capacity.

Fig. 5.5. Six types of a concentration-runoff or load-runoff relation according to Behrendt (1993). Top row: CQ functions. Bottom row: corresponding LQ functions.



5.11 The Adjustment Procedure

c_{ij} is the measured concentration of sample *j* in the year *i* , q_{ij} is the related runoff and

$$L_{ij} = c_{ij}\, q_{ij}$$

is the measured load. Further the CQ function $c_{ij}(q_{ij})$ obtained with one of the methods described above – Method N, H, L1,-L4, S1 or S2 – is also given, this function depicting concentration as dependent on runoff and possibly other variables. Firstly it should be checked whether statistically non-admissible extrapolations of the CQ function do not fall within a concentration range which is either above or below the range of the measured concentration. If this be the case then the CQ or LQ functions will have to be accordingly limited.

The CQ function may also be used to determine the *estimated load* (the LQ function)

$$L_{ije} = c_{ij}(q_{ij})\, q_{ij},$$

as well as the *mean load*

$$L_{ijm} = c_{ij}(q_{0ij})\, q_{0ij}.$$

with q_{oij} denoting the corresponding long-term monthly mean of the runoff, expressed in the unit m^3 /s.

On the basis of the measured load, the estimated load and the mean load, the (multiplicatively) adjusted load is finally calculated using the following formula:

adjusted load = measured load x mean load / estimated load

In formal terms, the adjusted load may be expressed as:

$$L_{ija} = \frac{L_{ijm}}{L_{ije}} L_{ij} = \frac{c_{ij}}{c_{ij}(q_{ij})} L_{ijm},$$

in other words, the adjusted load can be derived from the measured load by multiplying with the correction factor $\frac{L_{ijm}}{L_{ije}}$. In order to prevent unavoidable estimation errors from causing a distortion in the adjustment factor, the latter should be limited both at the upper and lower ends. However this would only be relevant if the runoff rate in a month is either extremely high or extremely low and the relative estimation error is accordingly extremely large. With limiting Factor 3 it may formally be established that $L_{ija} = \lambda_{ij} L_{ij}$ with the adjustment factor

$$\lambda_{ij} = \begin{cases} \frac{1}{3} & \text{if } \frac{L_{ijm}}{L_{ije}} < \frac{1}{3} \\ 3 & \text{if } \frac{L_{ijm}}{L_{ije}} > 3 \\ \frac{L_{ijm}}{L_{ije}} & \text{otherwise} \end{cases}$$

Alternatively, the adjusted load can also be derived from the mean load by multiplying with the factor $\left(\sum_j L_{ijm}\right) / \left(\sum_j L_{ije}\right)$.

5.12 Alternative Methods of Adjustment

5.12.1 Extension of the TRANSPOS Method (Method BC)

The calculations discussed in the following were carried out by Mr. Brunswig in Kiel, with the help of the TRANSPOS program. The method concerned is a semi-automatic method of calculation for real and standardized annual loads.

As per the approach generally adopted with TRANSPOS, standardized loads are determined as follows (refer also Brunswig 1994). First the entire body of values (c_{ij}, q_{ij}) for the entire series of measurements (i=index for the year, j=index of values within a year) is plotted on the CQ graph and the differential curve $c=f(q;s)$ averaged for the entire period under study adjusted with a semi-automatic method. Here, s denotes the season concerned. This CQ function, "mother function" of all measurement data, serves as a reference curve for separating individual intervals whose measurement points are not adequately represented by the reference curve. For this purpose a standardized coefficient

$$k_i = \frac{1}{m}\sum_{j=1}^{m}\frac{c_{ij}}{f(q_{ij}, s_{ij})}$$

is calculated for every year i in order to ascertain the years which could be clubbed together for calculating the CQ function. While determining the sum-total, all the measurement values of a hydrological year in each case shall be taken into account. In a second stage, the CQ functions of the sub-intervals are calculated. The calculation of annual loads standardized by runoff is undertaken with the help of the CQ function of the intervals whose construction includes the measurement values of the year j, with the same defined long-term distribution of runoff values in each case (long-term hydrograph). Thus differences in the standardized load value, which is based on the actual discharge values for the reference period, appear merely as a result of the different CQ functions of the intervals. They correspond with the varying dynamic states of the emission / immission system.

Since all the years of the interval concerned are always assigned the same standardized annual load value, it is not possible to subject these standardized load values, as per the fundamental approach outlined in Chapter 3, to a trend analysis based on the annual values in the following.

In order to reveal the individual fluctuations from year to year in the runoff-standardised annual loads, the averaged coefficients of position are once again calculated on the basis of the concept of multiplicative adjustment, with the CQ functions of the intervals $f_i(q,s)$ being used here instead of the overall CQ function.

$$k_i^* = \frac{1}{m}\sum_{j=1}^{m}\frac{c_{ij}}{f_i(q_{ij}, s_{ij})}.$$

If one multiplies this coefficient with these – as per TRANSPOS – runoff-standardised loads, one obtains a load value which is depicted with the symbol BC in the result charts. This load value is subject to random fluctuations from year to year so that a trend analysis on the basis of this value seems admissible (under certain conditions).

5.12.2 Standardisation of the OSPAR Load to the Long-Term Mean Runoff (Method A0)

If the annual load is approximately proportionate to the runoff it is recommended that the following load formula be used for an annual load value standardised to the long-term mean runoff:

$$L_i = 31{,}5576 \frac{MQ}{\frac{1}{m}\sum_{j=1}^{m} q_{ij}} \sum_{j=1}^{m} c_{ij} q_{ij} \, .$$

where MQ denotes the long-term mean runoff (m^3 /s). The unit of annual load thus ascertained corresponds with

- t/a if mg/l is used as the unit of measurement for the concentrations.
- kg/a if µg/l is used as the unit of measurement for the concentrations.

This method is referred to as A0 below. The advantage of this method lies in its extreme simplicity and in the fact that the annual loads obtained therefrom are only dependent on the data from the relevant random sample for the year. Further, unlike in Section 4.2, one need not proceed on the assumption that autocorrelations in the series of annual runoff induce substantial autocorrelations in the annual loads obtained.

However, a major disadvantage of the method lies in its application being advisable only in such cases in which load and runoff are more less proportionate. Otherwise one has to contend with a substantial overadjustment.

6 Aggregation of the Adjusted Loads

After the relevant adjusted load L_{ija} has been ascertained for every measurement time t_{ij} for which concentration values c_{ij} are available, one obtains the mean adjusted load in year i by calculating the arithmetical mean value and the adjusted annual load L_{ia} through a projection for the annual value:

$$L_{ia} = \frac{31{,}5576}{m} \sum_{j=1}^{m} L_{ija}$$

The unit of annual load ascertained in this manner corresponds

- with t/a where mg/l is used as the unit of measurement for the concentrations
- with kg/a where µg/l is used as the unit of measurement for the concentrations

It is assumed here that the underlying runoff values are determined in the unit of measurement m^3 /s.

The mean value is calculated on the basis of all values available for the relevant calendar year. Care should be taken in the process to ensure that the period under investigation is evenly covered, in other words it is assumed that the measurements are undertaken at regular intervals and that no extended period of time is left uncovered.

7 Trend Analysis

There is a wide range of statistical instruments available for the trend analysis of adjusted and non-adjusted annual values. For instance, the choice ranges from simple linear regression analyses to Mann-Kendall's non-parametric trend test and non-parametric smoothing methods. In the past the pros and cons of these methods gave rise to some controversies. If one compares the various methods for trend analysis it quickly becomes clear that each of these methods has its specific advantages and disadvantages. The suitability of a method would depend not only on the statistical distribution of the data but also on the purpose of the trend analysis. In this connection a distinction has been made by ICES WGSAEM between the following four functions of a trend analysis of annual values:

Visual representation of data by means of a trend line.	A visual representation through a trend line for instance serves on the one hand to summate all individual values and, on the other, to reveal anomalies such as outlines.
Statistical Trend Test	A statistical trend test serves to examine the question whether the trend can be taken to be statistically validated. If this is not the case, then there is nothing that dismisses the initial assumption that the fluctuations observed are but random alterations which are not caused by a systematic trend. Only when there is evidence of a statistically validated trend does a more far-reaching statistical evaluation of the time series appear meaningful from the statistical point of view.
Recording the linear trend component	The linear trend component allows the percentage reduction in inputs in a given period to be recorded.
A comparison of the present level with a reference level or the level at an earlier point of time.	Where a reference value or reference time is given, a trend analysis can be used to examine whether the current level is higher or lower than the reference value or whether there has been a rise or fall since the reference time.

The following sections will discuss in detail the various functions and appropriate analytical methods (a revised version of a text taken from ICES 1999). It is assumed here that a time series of annual values is available, although it is of no consequence whether or how the values had been adjusted.

7.1 Visual Representation of the Data with a Trend Line

A visual trend line not only enables a summation of data, but also facilitates visual comparison between different regions or contaminants if the relevant trend lines are represented in a diagram. With the help of suitably defined trend lines it may be visually established whether a general trend for various regions or contaminants prevails or to what extent there is evidence of specific differences. Additional information may be obtained by including confidence and prognostic ranges.

Smoothing methods such as cubic splines or the so-called LOESS smoother are suitable for visual representation whereas a simple polynomial regression results in a bad model adjustment in many cases. There are ultimately hardly any limits set to the choice of a method, for there is no statistical criterion which clearly favours a certain method. For recording trends in biota, WGSAEM recommends the LOESS smoother, based on a data window of 7 years, that is to say, every estimated value is based on data for 7 years in each case (for the relevant year as well as for the three preceding and the three subsequent years, with a modification of the data windows being necessary both at the beginning and at the end of the time series). This generally permits a favourable adjustment to the general course of the trend in the case of typical monitoring time series.

However the LOESS smoother on the cubic spline are not equally suitable for application in every case. If one has to contend with individual, extremely sharply deviating data values (yearly data), then there is the question as to whether these values should be incorporated with the full weight of their impact while determining the trend line or whether their influence should be reduced with a suitable robustification method. Figure 7.1 shows a trend line determined with a LOESS smoother for a hypothetical time series with a sharply deviating individual value in the year x=5. This sharply deviating value in x=5 'pulls' the entire trend line up, with the result that the trend line for the years x=3,4,6 and 7 runs above the individual values in each case. Where there is reason to assume that the sharply deviating individual value in the year x=5 does not represent actually prevailing conditions but is the result of a measurement error, it is recommended that the influence of the potential outlier be reduced through a suitable robustification of the smoothing process. This can be undertaken through an iterative application of a weighted smoothing method in which the weights are determined by the quantity of the residue in each case. The effect of such a robustified smoothing process in clearly shown in Figure 7.2. Obviously the value in the year x=5 has virtually no impact any longer, the result being a convex form of the trend function which is extremely well adjusted to the remaining individual values.

In each case, the pros and cons of a robustification of trend determination should be assessed. It is just as important to consider the underlying distribution of measurement errors as it is the question regarding the specific purpose of the trend calculations in each case. To date it has been non-robustified smoothing methods which have for the most part been used, one of the reasons for this however being that robustified smoothing methods are not so easy to handle from the statistical-methodical point of view and the calculation of confidence and prognostic margins remains unclear.

Figure 7.1

LOESS trend for a time series with a sharply deviating value.

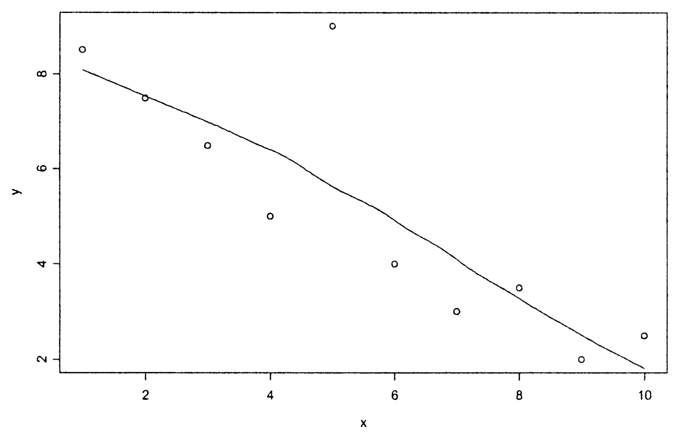
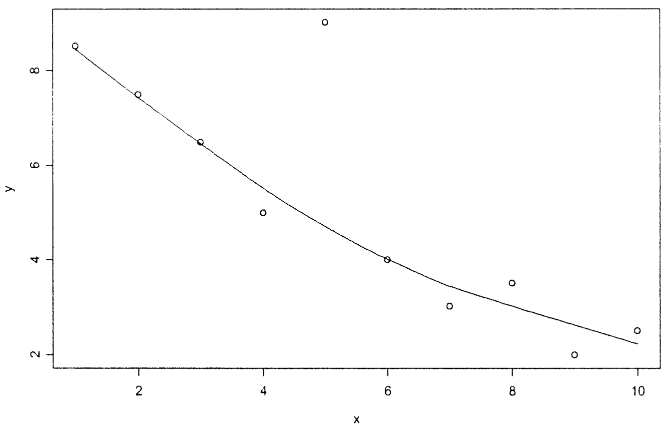


Figure 7.2

Robustified LOESS trend for a time series with a sharply deviating value.



7.2 Statistical Trend Test

As long as the time series is dominated by random fluctuations from year to year and there is no clear-cut trend that is recognizable, the determination of a trend line and the variables derivable therefrom are of questionable worth if it is not proved that real changes are observable in the trend course. This question should be examined with the help of a statistical trend test. Such a test is based on the initial assumption (zero hypothesis) that there is no systematic trend and that all fluctuations are caused by random changes in the individual values. Only when this initial assumption can be refuted by a suitable trend test for establishing a given error probability ALPHA (with ALPHA for the most part being fixed at 5%) can the trend in question be regarded as significant, in other words as validated.

The choice of a suitable trend test should necessarily rest on a number of aspects. This on the one hand concerns the question as to which types of systematic trends are of interest, that is to say, the question whether only linear trends are to be considered or even non-monotonic trends are to be included alongside monotonic once. Further, attention should be paid to whether the statistical distribution assumptions for the trend tests concerned have been met (for instance, normal distribution) and to what extent the test can be regarded as robust (outliers). And last but not least, the power or selectivity of a test, that is to say the probability with which an actually prevailing trend is recognized, should also be considered.

Where both monotonic and non-monotonic trends are to be investigated, a LOESS smoother-based test may be used. However where only monotonic trends are expected, Mann Kendall's test may be opted for. This is a non-parametric method that dispenses with the precondition of normal distribution.

7.3 Determination of the Linear Trend Component

Apart from the general (non-linear) trend line, the linear trend component in a given period of time is also of interest in many cases. This linear component can be expressed through the (positive or negative) gradient of the linear trend line or as the percentage rise or fall. Additionally, the indication of a confidence interval for the gradient parameter is also useful.

The gradient parameter can be determined through a linear regression by the LOESS smoother or Theil's non-parametric method with which the differences $(y_i-y_j)/(i-j)$ are first and foremost ascertained for all the years i and j, with annual data y_i and y_j and $i > j$. On the basis of this, the mean value is then constructed. Where outliers appear due to measurement errors, a robustification of the linear regression method may be opted for. One should be aware that the different methods could yield extremely divergent results especially in the case of sharply non-linear trend lines. Particularly for longer non-monotonic time series, the use of Theil slopes could lead to misleading results, with even a linear regression not necessarily generating a plausible result in the case of long time-series and sharply non-linear trends. Therefore, for long time-series with a clearly pronounced non-linear trend, it is recommended that a LOESS smoother be used.

7.4 Comparison with a Reference Level

Where a reference value or a reference time is available, a comparison can be made with the current level. For this, the difference between the prevailing level estimated on the basis of the trend line and the reference value or estimated level for the reference time is calculated. A statistical estimation of this difference will additionally require an estimation of the standard deviation of this difference or a confidence estimation. In addition to this a statistical test could be undertaken to check whether the difference ascertained deviates significantly from zero. Simulation calculations have however shown the selectivity of such a test to be unsatisfactory in many cases. This points to the fact that the methods of estimation used frequently give rise to substantial estimation errors Statistical methods should therefore necessarily be improved.

8 Power Function

8.1 Objective

The annual loads calculated with the OSPAR formula reveal year-to-year fluctuations which may be classified as follows:

- random fluctuations which may be attributed to varying runoff
- random fluctuations which may not be solely attributed to varying runoff (but for instance to anthropogenically conditioned runoff)
- random fluctuations caused by errors of measurement

In addition to this, there is a long-term systematic trend which is assumed to be anthropogenically conditioned (for instance by emission-control measures).

As explained earlier, the aim of the adjustment is to eliminate the *additional* random fluctuations in the annual loads caused by fluctuations in runoff, so as to maximize the sensitivity of the downstream trend-analysis method. Accordingly, an efficient method of adjustment ensures that the adjusted annual loads reveal minimal year-to-year fluctuations, that is to say, variations in values from year to year should be kept to the minimum. Naturally it must be ensured in the process that the other components of the random fluctuations do not get distorted, for this would make a statistically "clean" trend analysis of the adjusted annual loads impossible.

8.2 Measuring the Trend Sensitivity

In order to ascertain the extent to which an adjustment results in the increased trend sensitivity of the method as a whole, a measure of assessment that can be interpreted in simple terms is required. A measure for trend sensitivity that is interpretable in practical terms is the probability with which a hypothetical trend becomes statistically significant after a specified number of years. This probability as a function of trend intensity is designated the power function.

The power function depends on the expected time trend on the one hand and on the variability of the annual loads to be expected on the other. The year-to-year variability of annual loads can only be prognosticated, it being expedient here to assume that the variability that had occurred in the past would also occur in the future. This constitutes the central assumption of the so-called post-hoc power function where on the basis of certain statistical model assumptions the probability of a given trend being identified as statistically significant is calculated.

The post-hoc power is determined on the basis of the assumption that a linear trend is calculated with the LOESS smoother. The length of the period under investigation was put down to be n=10 years for calculations purposes. The post-hoc power is determined through the relative standard deviation of the annual loads the use of the standard deviation of the relative residues being recommended for this purpose.

8.3 Interpretation

The power functions is particularly useful for examining the suitability of a monitoring system for recording time trends. This is best explained with the help of the following example: Emission-control measures aiming at a 25% reduction in input within a period of 10 years, that is from 10000 t/a to 7500 t/a, are to be carried out. In this case one would ideally assume a linear reduction spread over the entire period, that is to say, an annual reduction of 250 t/a.

The value of the power function in the relevant case will indicate whether it is possible to statistically validate the reduction (with a prescribed level of significance) after the 10 year period, on the basis of the existing monitoring system. The power function indicates the estimated probability for a statistical validation of input reduction. Where the value of the power function is greater than 0.9, it may be assumed that the existing monitoring system is well-suited for checking the efficacy of the measures undertaken. Where values are below 0.9 it is recommended that the monitoring system be improved either through a modified sampling process or through appropriate statistical methods, such as adjustment methods for instance, in order to prevent the possibility of a validation of the reduction achieved proving unsuccessful despite the successful implementation of emission reduction.

As a rule, the power function depends on the trend assumed for the period under investigation, though where trend tests based on the smoother are used, the results obtained for the linear trend are more or less valid for the non-linear, monotonic and 'smooth' trends too.

Further, it should be pointed out that the power function is essentially dependent on the variability of the annual values in the past. But given the fact that this variability itself is subject to random influences, it must be assumed that even future variability can be higher or lower than that assumed. Thus the power function itself can only be regarded as an estimation and not as a fixed, constant figure. Besides, the shorter the period, the greater the extent to which this estimation is influenced by random errors. It is therefore recommended that the data series drawn upon be as long as possible, or that the power function be ascertained for a variety of potential variability values so as to make the influence of this variability on the result discernible.

9 Assessment of the Results

9.1 Analysis of the Adjusted Annual Loads

The methods discussed in this project these being

N	= non-parametric smoothing as per Stalnacke
H	= use of Hebbel's method of estimation
L1	= local regression with season
L2	= local regression with season and lagged runoff effect
L3	= local regression with season, temperature and lagged runoff effect
S1	= estimation with local splines
S2	= estimation with local splines
BC	= extension of the TRANSPOS method (Brunswig)
A0	= standardising the OSPAR-load to the long-term mean runoff

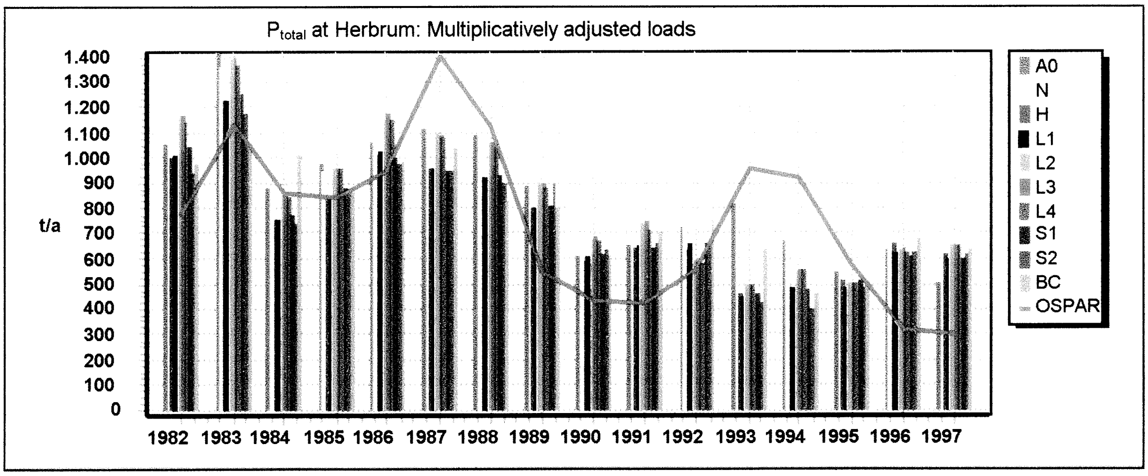
were investigated using the measurement series for Pb, Cd, P_{total}, PO_4-P, NH_4-N, NO_3-N and suspended matter in the River Rhine at Lobith and the River Ems at Herbrum. Measurements in the Rhine were undertaken at fortnightly intervals while those for the River Ems were done once a month. In addition to these series, the temperature and daily runoff series were also available.

The aim of the investigation presented below was to test the performance of the methods under real conditions, that is to say, with sharply divergent time series, values close to the limit of determination or detection, values with only one significant digit, outliers and such like. In the process the methods were deliberately not adjusted individually to each time series since this would in any case hardly be possible in actual practice. As per this objective, preference is to be given to that method which is particularly simple and which yields values that are acceptable for all parameters.

Appendix A contains a graphic representation of the calculated annual loads and the mean yearly concentrations together with the corresponding LOESS trends. These graphic shall be explained by the results for P_{total} at Herbrum:

The representation of the multiplicatively adjusted loads (Fig.9.1) for each year consists of nine bars, which refer to the adjusted annual loads of the methods A0, H, H, L1, L2, L3, L4, S1, S2 and BC. The solid line represents the annual load according to the OSPAR formula.

Figure 9.1



The trends calculated with these annual loads are represented in Fig.9.2. The assignment of colors corresponds to the representation in Fig.9.1, but line and bar have been changed. The bars represent the calculated trend for the OSPAR load, whereas the solid lines represent the trend for the several adjustment methods (LOESS trend). Partly the trends of the several methods cover each other. The sequence equals the sequence in the legend, i.e. the trend for method A0 is covered by the trend lines of all other methods, whereas the trend line for method BC covers all other methods.

Figure 9.2

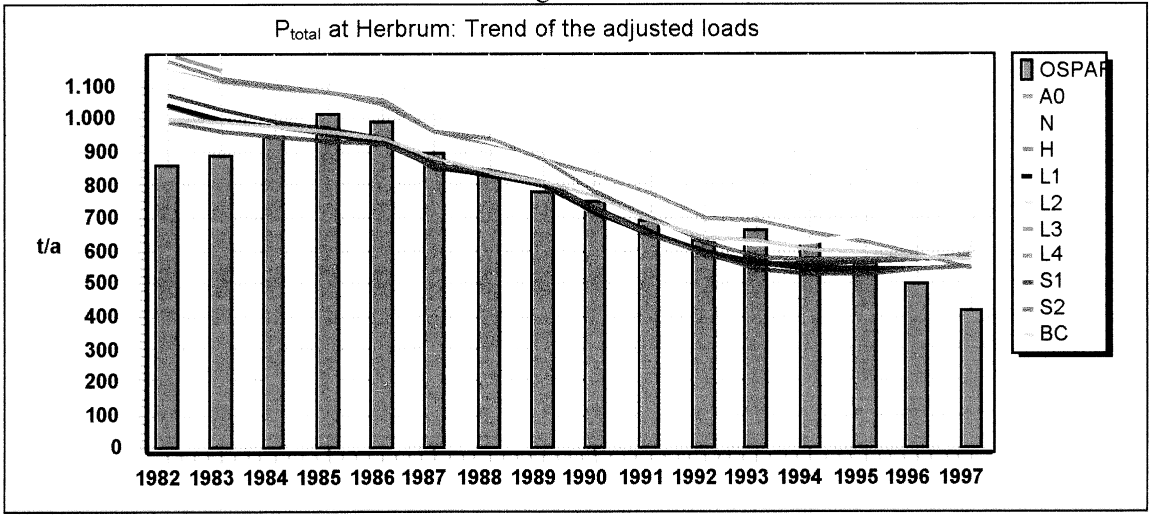
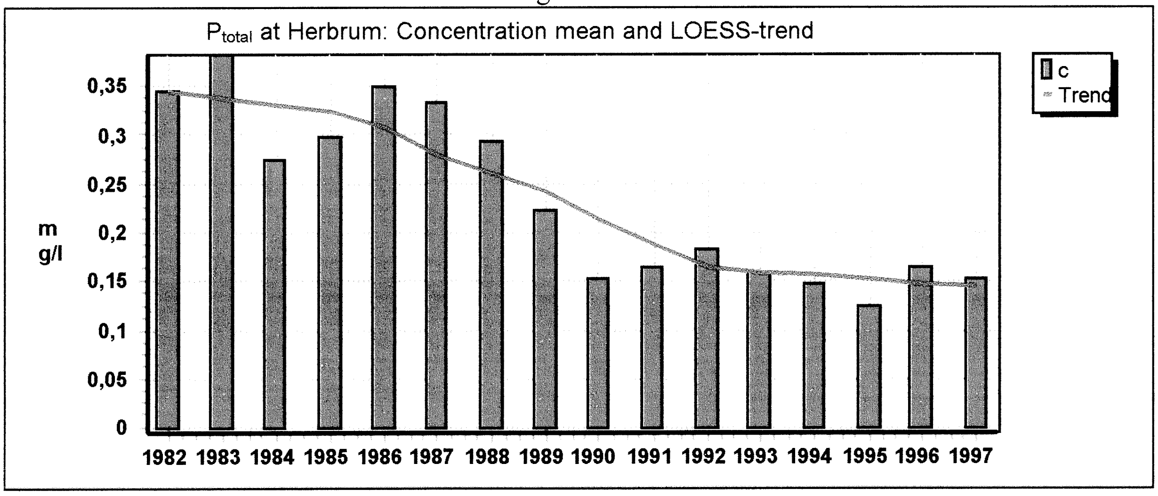


Figure 9.3



9.1.1 Results for the River Ems at Herbrum

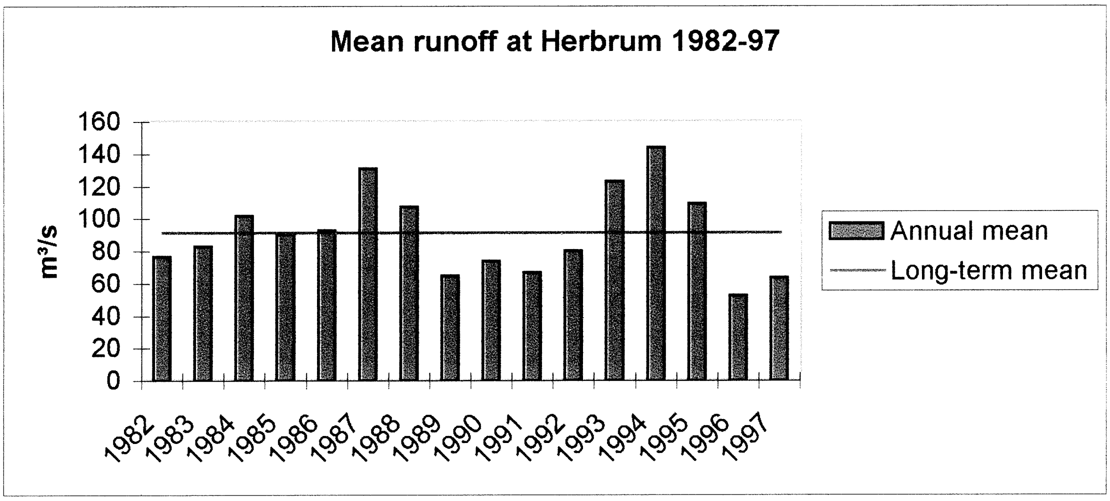
Pb at Herbrum

Since the data available only covers a period of five years, the minimum prerequisites for an adjustment cannot be considered as met. Nonetheless the results do show a relatively good correspondence for all the adjustment methods if one excludes Method A0 and Method N from consideration. In the present case, the latter method does not permit an acceptable adjustment of the LQ-function due to the short span of the period under observation. With the exception of

Methods A0 and N, all the other adjustment methods show slightly upward trends as the mean concentration values, whereas the OSPAR load gets clearly reduced over time.

This is attributable to the sharp reduction in runoff quantities during the period under investigation (see Figure 9.1) as well as to the runoff weighting factor in the OSPAR formula which has an added impact.

Figure 9.4



If the measured concentration had remained constant for all the measurements during the period concerned, there would have been a more than two-thirds reduction in the OSPAR load (-67%) between 1993 and 1997, given an adjustment of a linear regression straight line. This is in accord with the finding that the trend line for the OSPAR load for Pb shows a reduction of approximately 64% whilst the measured concentrations record a slight increase.

This result goes to show that OSPAR loads are wholly unsuited for trend analyses, at least for short time periods due to severe fluctuations in runoff.

Cd at Herbrum (Annex A3)

As in the case of Pb, for Cd too the data available only covers a period of five years. It is therefore not surprising that those adjustment methods which are particularly complicated and consequently necessitate larger quantities of data reveal the most unfavorable characteristics. What is referred to here are the Methods N, H and L4 which do not prove satisfactory with regard to the adjustment of the CQ or LQ function. Due to structural reasons Method A0 also yields results that are not acceptable. The remaining Methods L1, L2, L3, S1 and S2 also yield more or less similar results. All the results are conditioned by a drastic rise in concentrations for the year 1997. It is for this very reason that the OSPAR loads too register a smaller reduction, whereas the adjusted loads on the other hand are characterized by a more markedly upward trend. However it has been established that this trend is solely attributable to the result for the year 1997 and that no statistically significant trend can be proved.

P_{total} at Herbrum (Annex A4)

With the exception of Method A0, all the adjustment methods for P_{total} are relatively close to each other and tally well with the mean concentration values. Once again, the OSPAR load yields clearly deviating results with two extreme values for the years 1987 and 1993/94, the reason for this being the markedly higher mean runoff values for these years. Of particular note is the fact that the adjusted loads have remained more or less constant since 1993 whilst the OSPAR load undergoes a sizable reduction owing merely to the increased runoff values for the years 1993/94.

PO_4-P at Herbrum (Annex A5)

For PO_4-P too, all the adjustment methods with the exception of Method A0 are relatively close to each other and tally well with the mean concentration values. Again clearly deviating results with extreme values for the years 1993/94 are recorded for the OSPAR load, the cause for this being the markedly higher mean runoff values. However, of particular note here as against P_{total} is the finding that there is an extremely sharp reduction in loads of more than 50% for the period between 1986 and 1987, this reduction being even more pronounced for the adjusted loads than for the OSPAR load.

The percentage reduction in loads for the period between 1986 and 1995, ascertained on the basis of the trend lines, varies between 26% and 45% depending on the method, while an examination of the OSPAR loads and the mean concentration values revealed a somewhat higher reduction. Behrendt et al (1999) have obtained an emission-related reduction of 50.1% (discharge-corrected: 45%) from point and diffuse sources for the entire catchment area.

NH_4-N at Herbrum (Annex A6)

In the case of NH_4-N, the OSPAR load for 1987 is a conspicuous "outlier". Essentially, this value may be attributed to flood conditions prevailing in January 1987: At 2mg/l the corresponding NH_4-N concentration for January 1987 amounts to three times the annual mean while the corresponding runoff value of 695 m^3/s exceeds the long-term mean seven fold. This high-water period causes the OSPAR load to increase by over 100%. This should not be looked upon as something particularly unusual, for during high-water conditions up to 90% of the annual load can be discharged into the sea depending on the water level.

Characteristically, the adjusted loads are only marginally affected by this. With the exception of Method A0, all the adjustment methods are relatively close to each other and also tally well with the mean concentration values. The trend lines of the adjusted loads for the period 1993-1997 indicate a reduction of approx. 20-30%.

NO_3-N at Herbrum (Annex A7)

In the case of NO_3-N, all the adjustment methods yield results that are relatively close to each other while the OSPAR load again records clear deviations and substantial year-to-year fluctuations. It is owing to the clear drop in the mean runoff from 1993 to 1997 that the trend line of the OSPAR load indicates a reduction of over 30% for the entire period, whereas the trend line of the adjusted loads as well as of the mean concentrations points to a reduction of approximately 10%.

Suspended Matter at Herbrum (Annex A8)

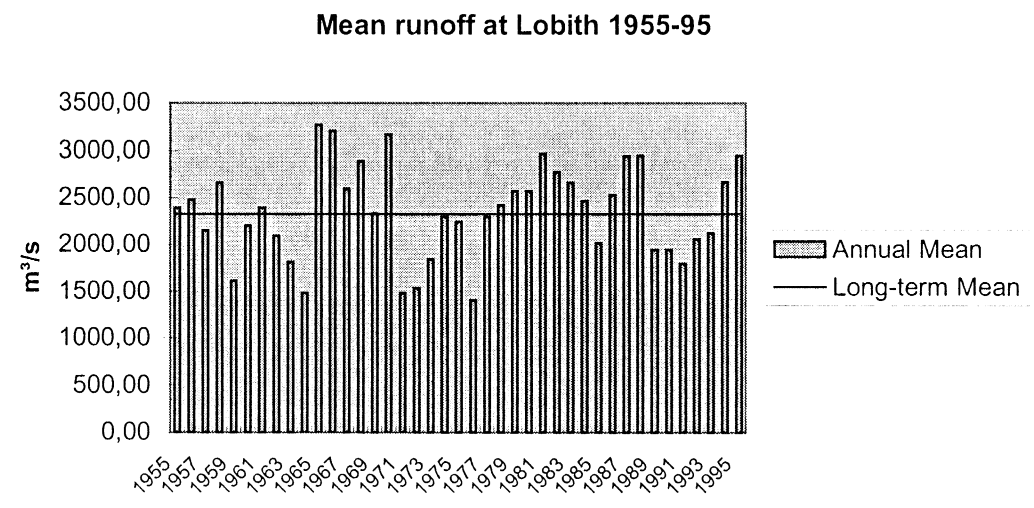
For suspended matter all the adjustment methods with the exception of Method A0 yield results close to each other while the OSPAR load shows clear deviations. There is no clear trend discernible.

9.1.2 Findings for the River Rhine at Lobith

Pb at Lobith (Annex A9)

While both the adjusted Pb loads as well as the mean concentration values show a uniformly downward trend from 1991, the trend for the OSPAR load is perceptibly upward from 1992, this being attributable to a rising mean runoff in the period 1992-1995 (Figure 9.5).

Figure 9.5



Cd at Lobith (Annex A10)

For the eighties it was found that the adjusted loads sharply decreased by about 90%, this decrease being accompanied by sharp fluctuations form year to year. From the early nineties onwards a further slight decrease in the adjusted loads may be found. As against this, an upward trend is again discernible for the OSPAR load from 1993. Within the group of adjusted loads, Methods S1 and S2 reveal a deviating behaviour as does the semi-automatic Method BC.

Basically, the mean concentration values reveal a behaviour similar to that of the adjusted loads, although the yearly fluctuations in the values were somewhat greater as a result of the concentrations not being adjusted.

P_{total} at Lobith (Annex A11)

For P_{total} too, all the adjustment methods except Method A0 prove to be relatively close to each other and tally well with the mean concentration values. The results for the OSPAR load are slightly deviating. What is conspicuous is the clearly wider fluctuation range for the mean concentration values and the OSPAR load, which makes an assured trend determination difficult. For all the methods, the estimated percentage reduction in inputs for the period 1986-95 is around 70% which tallies well with the emission-related reduction rates of 67,9% obtained by Behrendt et al (1999) for the point and diffuse sources of the Rhine catchment area.

PO_4-P at Lobith (Annex A12)

For PO_4-P too, all the adjustment methods with the exception of Method A0 yield results which are relatively close to each other and tally well with the mean concentration values as well as with the results for the OSPAR load, although the fluctuation range for the adjusted loads is on the whole somewhat smaller. A reduction in loads of up to 80% is obvious for all the methods from 1985.

NH_4-N at Lobith (Annex A13)

In the case of NH_4-N there were sizable differences between the methods investigated, with particularly the period between 1960 and 1975 registering an extremely volatile trend where the mean concentration values in particular show extremely sharp fluctuations. With the exception of the OSPAR load, all the trends point in a direction that is markedly downward at the end of the time series in 1995, with a reduction of about 70% being ascertainable from 1986.

NO_3-N at Lobith (Annex A14)

For NO_3-N, all the adjusted loads investigated yield values close to each other and tally very well with the mean concentration values in their trend. The OSPAR load on the other hand produces extremely sharp deviations expressed inter alia by the fact that except for the OSPAR load all the trends for the year 1995 point downward. Besides, what is conspicuous are the extremely severe year-to-year fluctuations of the OSPAR load.

Suspended Matter at Lobith (Annex A15)

For suspended matter there are significant differences between the methods. A clear trend cannot be observed. However, due to the length of the time series of only five years it cannot be expected to detect any significant trend.

9.2 Variability of the Adjusted Annual Loads

Besides the direct comparison of the adjusted load value, the variability of the annual load values constitutes the main criterion of assessment of the various adjustment methods. Due to extremely marked differences in level over long periods of time this variability is calculated by the relative deviation of the annual values from the corresponding LOESS trend. Table 9.1 presents an overview of the standard deviations of these relative deviations expressed as a percentage of the corresponding level. The length of the time series varies between 5 and 41 years. It may be noted that for series of less than 10 years, the standard deviations are subject to sharp random fluctuations.

Alongside the standard deviations themselves, the quotient S_{Ratio} of the standard deviations for the adjusted load and the standard deviation of the OSPAR load is important. Thus in the case of sufficiently long measurement series the period of investigation at a given total input reduction can be reduced by the factor S_{Ratio} through the use of adjusted annual loads in order to obtain the same trend sensitivity which would otherwise be obtained with the OSPAR load. S_{Ratio} may also be understood as that factor by which the standard error of the trend assessment gets reduced if an adjusted load is used instead of a non-adjusted load.

Table 9.2 contains a representation of the quotient S_{Ratio} for all the adjustment methods covered by this project. Particularly in the case of NO_3-N, an adjustment enables a substantial improvement in the trend sensitivity which would otherwise only have been possible if the period of measurement were increased by the factor 2.5 (Ems) or the factor 4 (Rhine). In the case of the other nutrients the gains in efficiency are not so substantial although even here a 25-60% reduction in standard deviation is to be expected if one excludes NH_4-N in the Rhine for which special factors may possible have had an effect particularly in the period up to 1970. In the case of heavy metals no clear assessment is possible since only the data for five years could be used for the Ems. However, for the Rhine, an adjustment with Cd makes a clear-cut reduction in the standard error possible whereas no positive effects are discernible for Pb. A more detailed examination of the residues reveals some sharply deviating values which cannot be explained by the CQ function, though they have a substantial impact on the variability of the annual loads. The two abovementioned tables contain the results of the CQ function determined through the Transpos model (BC). It should be noted here that the loads calculated with the Transpos model essentially reveal a trend which is similar to that of the adjusted loads. However a direct comparability of the results is not assured since the adjustment of the CQ function does not occur automatically in the Transpos model.

Besides the abovementioned characteristic values, the power is also taken into consideration for recording a trend taken as relevant. Presented in Tables 9.3 and 9.4 are those power values used for fixing a hypothetical trend which leads to a 20-30% load reduction over a period of 10 years. The power is calculated on the basis of the standard deviation of the relative residues given in Table 9.1.

In the case of the Rhine, the use of adjusted loads, as against the OSPAR load, makes a sizable improvement in trend sensitivity possible for NO_3–N, P_{total}, PO_4-P, Cd and suspended matter, while only marginal differences are to be found for NH_4-N, with even a slight deterioration in trend sensitivity being recorded for Pb. On the other hand the use of mean concentration values results in a considerable deterioration in the power. Only in the case of NO_3-N and suspended matter does the use of mean concentration values bring off an improvement as compared to the OSPAR load.

In the case of the Ems, the use of adjusted loads instead of the OSPAR load improves the trend sensitivity for all nutrients. Even the mean concentration values make a substantial improvement in trend sensitivity possible, the trend sensitivity obtained here lying within the range of that obtained with adjusted loads. This may however be attributed to the heavy seasonal fluctuations in the runoff for the Ems. Thus, the long-term monthly mean runoff in January is more than five times that in August. Consequently, the variability in load values (both for the OSPAR as well as the adjusted loads) is to a large extent conditioned by the variability of the measured concentrations during the winter half of the year. Due to the fact that the mean yearly concentration is equally influenced by all the measurements, the fluctuations in this case may be expected to be considerably smaller, However, since the trend of concentration values in the case of strong seasonality does not necessarily reflect the trend in inputs, the use of mean concentration values for assessing the efficiency of reduction measures does not seem advisable.

On the whole it may be noted that firm evidence of reduction (ie. at a power of at least 90%) for a reduction rate of 20%within a period of 10 years can only be assured for NO_3-N in the Rhine and that too only when adjusted loads are used. At a reduction rate of 50%, firm proof of reduction is guaranteed for NO_3-N and, to a lesser degree, for P_{total}, PO_4-P and Pb (only in the Rhine). For Cd and NH_4-N, firm proof of reduction is not assured either for the Rhine or for the Ems even at a reduction rate of 50%. In the case of the Ems, it is advisable – in view of a marked seasonality in runoff – to use a modified sampling concept with a higher sampling frequency in winter (and, if need be, reduced sampling during the summer months) in order to improve the detectability of the reduction measures.

Table 9.5 presents the reduction values calculated for the various methods during the period 1985-95. A comparison of the results shows that in a whole series of cases the OSPAR load clearly deviates from both the results for the average yearly concentration as well as from the adjusted loads. One of the reasons for the difference not being even greater is that the time series investigated are to an extent extremely long.

Table 9.1: Relative standard deviation

Station	Parameter	Time series	Concentration	OSPAR	A0	N	H	L1	L2	L3	L4	S1	S2	BC
Lobith	NO_3-N	55–95	6,6%	20,7%	6,6%	5,1%	5,2%	5,1%	4,9%	5,0%	5,0%	6,2%	6,4%	6,2%
Lobith	NH_4-N	55–95	24,0%	16,0%	23,4%	16,0%	15,9%	16,2%	15,3%	15,5%	15,1%	15,7%	17,0%	16,4%
Lobith	P_{Total}	73–95	13,1%	11,7%	13,8%	8,7%	9,2%	8,9%	8,3%	8,9%	8,9%	9,7%	10,1%	8,8%
Lobith	PO_4-P	73–93	17,2%	20,4%	18,4%	13,8%	14,9%	14,1%	14,6%	14,4%	15,7%	17,7%	15,7%	12,6%
Lobith	Cd	82–95	29,1%	29,9%	28,6%	28,8%	24,9%	24,2%	24,0%	22,8%	24,1%	23,7%	31,1%	
Lobith	Pb	82–95	16,3%	14,2%	15,9%	15,5%	15,8%	15,0%	15,3%	15,3%	15,1%	17,1%	14,5%	17,8%
Lobith	Suspended matter	91–95	7,3%	22,2%	26,0%	75,6%	14,0%	9,5%	6,4%	7,2%	5,9%	9,7%	8,5%	
Herbrum	NO_3-N	82–97	8,6%	24,6%	13,7%	13,8%	9,4%	9,4%	9,3%	9,6%	9,6%	12,4%	14,6%	13,1%
Herbrum	NH_4-N	82–97	31,0%	55,3%	36,1%	25,3%	25,3%	32,9%	33,6%	34,3%	34,0%	27,3%	30,2%	
Herbrum	P_{Total}	82–97	15,8%	37,6%	17,4%	16,8%	15,6%	15,8%	14,9%	14,9%	14,6%	14,4%	16,4%	14,4%
Herbrum	PO_4-P	84–97	30,7%	51,4%	34,4%	30,2%	27,1%	27,1%	26,6%	27,4%	26,9%	30,1%	26,5%	20,9%
Herbrum	Cd	93–97	78,5%	33,7%	25,5%	55,1%	39,6%	42,9%	46,9%	48,7%	58,2%	49,3%	50,0%	58,8%
Herbrum	Pb	93–97	7,3%	22,2%	26,0%	75,6%	14,0%	9,5%	6,4%	7,2%	5,9%	9,7%	8,5%	35,5%
Herbrum	Suspended matter	82–97	19,2%	31,8%	29,7%	20,1%	19,9%	20,6%	20,0%	20,4%	20,2%	19,3%	22,4%	26,2%

Table 9.2: S_{Ratio} (Ratio of standard deviation of adjusted load and standard deviation of OSPAR load)

Station	Parameter	Time series	$\sqrt{1-\rho^2}$	Concentration	A0	N	H	L1	L2	L3	L4	S1	S2	BC
Lobith	NO_3-N	55–95	51,10%	31,88%	31,88%	24,64%	25,12%	24,64%	23,67%	24,15%	24,15%	29,95%	30,92%	29,95%
Lobith	NH_4-N	55–95	96,60%	150,00%	146,25%	100,00%	99,38%	101,25%	95,63%	96,88%	94,38%	98,13%	106,25%	102,50%
Lobith	P_{Total}	73–95	81,50%	111,97%	117,95%	74,36%	78,63%	76,07%	70,94%	76,07%	76,07%	82,91%	86,32%	75,21%
Lobith	PO_4-P	73–93	95%	84,31%	90,20%	67,65%	73,04%	69,12%	71,57%	70,59%	76,96%	86,76%	76,96%	61,76%
Lobith	Cd	82–95	90%	97,32%	95,65%	96,32%	83,28%	80,94%	80,27%	76,25%	80,60%	79,26%	104,01%	
Lobith	Pb	82–95	95,50%	114,79%	111,97%	109,15%	111,27%	105,63%	107,75%	107,75%	106,34%	120,42%	102,11%	125,35%
Lobith	Suspended matter	91–95	98,40%	32,88%	117,12%	340,54%	63,06%	42,79%	28,83%	32,43%	26,58%	43,69%	38,29%	11,8%
Herbrum	NO_3-N	82–97	51,80%	34,96%	55,69%	56,10%	38,21%	38,21%	37,80%	39,02%	39,02%	50,41%	59,35%	53,25%
Herbrum	NH_4-N	82–97	70,60%	56,06%	65,28%	45,75%	45,75%	59,49%	60,76%	62,03%	61,48%	49,37%	54,61%	
Herbrum	P_{Total}	82–97	62%	42,02%	46,28%	44,68%	41,49%	42,02%	39,63%	39,63%	38,83%	38,30%	43,62%	38,30%
Herbrum	PO_4-P	84–97	60,50%	59,73%	66,93%	58,75%	52,72%	52,72%	51,75%	53,31%	52,33%	58,56%	51,56%	20,9%
Herbrum	Cd	93–97	94,30%	232,94%	75,67%	163,50%	117,51%	127,30%	139,17%	144,51%	172,70%	146,29%	148,37%	58,8%
Herbrum	Pb	93–97	86,90%	32,88%	117,12%	340,54%	63,06%	42,79%	28,83%	32,43%	26,58%	43,69%	38,29%	159,91%
Herbrum	Suspended matter	82–97	85,40%	60,38%	93,40%	63,21%	62,58%	64,78%	62,89%	64,15%	63,52%	60,69%	70,44%	82,39%

Table 9.3: Power for 20 % input reduction within 10 years

Station	Parameter	Time series	Concentration	OSPAR	A0	N	H	L1	L2	L3	L4	S1	S2
Lobith	NO_3-N	55–95	80%	20%	80%	94%	93%	94%	95%	95%	95%	84%	82%
Lobith	NH_4-N	55–95	17%	27%	17%	27%	27%	27%	29%	28%	29%	28%	25%
Lobith	P_{Total}	73–95	35%	41%	33%	60%	66%	58%	63%	58%	58%	52%	49%
Lobith	PO_4-P	73–93	25%	20%	23%	33%	30%	32%	30%	31%	28%	28%	37%
Lobith	Cd	82–95	14%	14%	14%	14%	16%	17%	17%	18%	17%	17%	13%
Lobith	Pb	82–95	26%	31%	27%	28%	27%	29%	29%	29%	25%	31%	24%
Lobith	Suspended matter	91–95	33%	12%	16%	60%	24%	27%	24%	16%	12%	23%	78%
Herbrum	NO_3-N	82–97	61%	17%	33%	33%	54%	54%	55%	53%	53%	38%	30%
Herbrum	NH_4-N	82–97	13%	9%	12%	16%	16%	13%	12%	12%	12%	15%	14%
Herbrum	P_{Total}	82–97	27%	11%	24%	25%	28%	27%	30%	30%	30%	31%	26%
Herbrum	PO_4-P	84–97	13%	9%	12%	14%	15%	15%	15%	15%	15%	14%	15%
Herbrum	Cd	93–97	8%	12%	16%	9%	11%	10%	10%	10%	9%	10%	9%
Herbrum	Pb	93–97	73%	18%	16%	7%	32%	53%	82%	74%	87%	52%	61%
Herbrum	Suspended matter	82–97	22%	13%	14%	21%	21%	20%	21%	20%	20%	21%	18%

Table 9.4: Power for 50 % input reduction within 10 years

Station	Parameter	Time series	Concentration	OSPAR	A0	N	H	L1	L2	L3	L4	S1	S2
Lobith	NO_3-N	55–95	100%	63%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Lobith	NH_4-N	55–95	53%	82%	54%	82%	82%	81%	85%	84%	86%	83%	78%
Lobith	P_{Total}	73–95	93%	97%	91%	100%	100%	100%	100%	100%	100%	99%	99%
Lobith	PO_4-P	73–93	77%	64%	72%	91%	87%	90%	88%	88%	83%	83%	95%
Lobith	Cd	82–95	41%	39%	42%	41%	50%	52%	53%	56%	52%	54%	37%
Lobith	Pb	82–95	81%	89%	82%	84%	86%	85%	85%	86%	77%	88%	75%
Lobith	Suspended matter	91–95	91%	32%	50%	100%	75%	81%	76%	48%	30%	73%	100%
Herbrum	NO_3-N	82–97	100%	51%	91%	91%	100%	100%	100%	100%	100%	95%	88%
Herbrum	NH_4-N	82–97	38%	18%	31%	49%	49%	35%	34%	33%	33%	45%	39%
Herbrum	P_{Total}	82–97	83%	29%	76%	79%	84%	83%	87%	87%	88%	88%	80%
Herbrum	PO_4-P	84–97	38%	20%	33%	39%	45%	45%	46%	44%	45%	39%	46%
Herbrum	Cd	93–97	13%	34%	49%	19%	27%	25%	22%	21%	17%	21%	21%
Herbrum	Pb	93–97	100%	58%	48%	14%	90%	100%	100%	100%	100%	99%	100%
Herbrum	Suspended matter	82–97	69%	36%	40%	65%	66%	64%	66%	64%	65%	69%	58%

Table 9.5: Estimated reduction of inputs 1986-95 (for PO_4-P at Lobith: 1986-93)

Station	Parameter	Time series	Konzentration	OSPAR	A0	N	H	L1	L2	L3	L4	S1	S2	Emission[1]
Lobith	NO_3-N	55–95	22%	13%	19%	18%	25%	20%	20%	20%	20%	23%	20%	29,8%
Lobith	NH_4-N	55–95	72%	63%	66%	73%	43%	70%	71%	71%	71%	69%	68%	
Lobith	P_{Total}	73–95	73%	65%	68%	70%	72%	71%	72%	70%	70%	70%	76%	67,9%
Lobith	PO_4-P	73–93	75%	84%	73%	77%	76%	78%	80%	81%	80%	78%	74%	
Lobith	Cd	82–95	85%	81%	83%	85%	87%	84%	83%	84%	83%	83%	93%	
Lobith	Pb	82–95	30%	14%	20%	29%	33%	30%	27%	27%	27%	32%	38%	
Lobith	Suspended matter	91–95												
Herbrum	NO_3-N	82–97	20%	34%	20%	5%	18%	14%	13%	13%	13%	7%	5%	5,5%
Herbrum	NH_4-N	82–97	46%	70%	63%	55%	55%	42%	45%	43%	44%	41%	51%	
Herbrum	P_{Total}	82–97	48%	53%	43%	26%	45%	39%	39%	39%	39%	36%	36%	50,1%
Herbrum	PO_4-P	84–97	73%	71%	70%	64%	68%	68%	68%	67%	67%	70%	70%	
Herbrum	Cd	93–97												
Herbrum	Pb	93–97												
Herbrum	Suspended matter	82–97	-27%	-7%	-30%	-39%	-39%	-31%	-31%	-30%	-29%	-41%	-44%	

[1] Reduction rates for inputs in German basins in 1983-1987 and 1993-1997 for N_{total} und P_{total} (Behrendt et al 1999).

9.3 Selection of a Practicable Method of Adjustment

The following criteria shall apply during the selection of an adjustment method:

- Simplicity/rapidity of the algorithm: simplicity and rapidity are rated 1=very good, 2=good, 3=satisfactory, 4=adequate, 5=unsatisfactory.
- Data requirements: the method is more highly rated where the demands made on the data are low (school grades). Minus points shall apply where the data has to be presented as monthly data (Method N) or where additional data such as the runoff of the previous day or the water temperature are required (Methods L2, L3 and L4).
- Robustness under unfavorable conditions (absence of data, outliers, short data series).
- Trend sensitivity or variability in annual values: A high trend sensitivity is assured when the variability in annual values is as small as possible. For this the mean value of S_{Ratio} is determined through all 14 time series, that is to say both with the 7 parameters measured in the Ems as well as with the 7 measured in the Rhine (Table 9.2).
- Trend sensitivity or variability in annual values for the nutrients: In order to determine the suitability of adjustment methods particularly for nutrient loads, the mean value of S_{Ratio} is also determined for the 8 nutrient time-series (NO_3-N, NH_4-N, P_{total} and PO_4-P for the Rhine and the Ems in each case).

The evaluation results in terms of simplicity, data requirements and robustness as presented in Table 9.6 reflect the author's subjective assessment. However, the semi-automatic Method BC could not be taken into consideration due to the absence of a direct basis of comparison, given varying demarcations of the year and varying lengths of the time series considered in each case. Besides, the Method BC does not permit a fully automatic calculation but on the other hand necessitates the manual intervention of the evaluator.

If one compares the methods on the basis of variability, what strikes one first and foremost is the extremely high variability in annual loads for Method N, the mean variability of which exceeds the variability of the OSPAR loads. This may be explained by the fact that Method N is not suitable for extremely short series with a length of just five years and that it can get very unstable. On the other hand, the use of mean concentration values or Method A0 yields results that are clearly better, though the exceptions confirm the rule, as in the case of the results for NH_4-N and P_{total} at Lobith. In this connection it may be noted that as against other methods of adjustment, Method A0 obviously generates values that deviate as a rule. This is at the same time plausible given the fact that Method A0

- is not a method of adjustment that has a bearing on the individual load value but on the other hand effects a standardization in annual load and
- standardization rests on the implicit underlying assumption that there is proportionality between runoff and load whereas the relation between load and runoff in the case of all other methods is empirically determined from the data itself.

In terms of variability, Methods L1 – L4 as well as Method H prove to be suitable without exception in the sense that the difference vis-à-vis the best method in terms of variability in each case is not very large. However Method H is far more complicated in its computation than L1 – L4 and one may conclude therefore that a higher degree of complexity in computation does not pay off. The disadvantage with Methods L2 – L4 is that in addition to the runoff values on the day of measurement the runoff values for the previous day are required, as also the water temperatures in the case of Methods L3 and L4. While the inclusion of the water temperature obviously does not pay off, the consideration of the previous day's runoff in Method L2 effects a slight further improvement in trend sensitivity. However one disadvantage with Method L2 as compared to Method L1 is a lesser degree of robustness.

Table 9.6 : Evaluation of Adjustment Methods

Method	Degree of simplicity	Data requirements	Robustness	Variability (total)	Variability(nutrients)
Mean concentration value	*1= very good, 2=good, 3= satisfactory 4= adequate, 5=unsatisfactory*			*Variability of the OSPAR load = 100%*	
Mean concentration value	1	1	1	82%	71%
A0 (standardized to a long-term mean runoff)	1	1	1	88%	78%
N (Stalnacke)	3	3	4	113%	59%
H (Hebbel)	4	1	3	68%	57%
L1 (with season)	2	1	2	66%	58%
L2 (with previous-day runoff and season)	2	2	3	64%	56%
L3 (with temperature and previous-day runoff)	2	3	3	66%	58%
L4 (with temperature, previous-day runoff and season)	2	3	4	67%	58%
S1 (spline)	4	1	4	71%	62%
S2 (spline, local	4	1	4	72%	64%

It should however be noted that the above conclusions are for the most part valid for nutrients. Thus, given the extremely short time series for Pb and Cd, there can be no assessment for the heavy metal parameters, especially since the possibility of heavy-metal data being misrepresented due to a change in the analytical method or to specific analytical problems cannot be ruled out.

10 Recommendations

For calculating anthropogenic trends in nutrient loads it is recommended that adjusted loads be used as an experiment on a broad basis. In the process, preference should be given to Method L1 where simplicity and robustness of method are the main criteria of selection. An adjustment on the basis of a specifically adjusted statistical model is recommended for more detailed examinations of individual rivers with regard to reduction measures. Particularly in the case of "difficult" parameters with extremely variable discharges and extreme runoff levels, a markedly non-linear LQ function, heavy wash-off effects or temporally abrupt changes in the LQ function, an individually adjusted evaluation has advantages over an automatic process.

Due to the short series and possible chemical-analytical problems, a final recommendation with regard to the adjustment of heavy metal loads cannot be made at this stage. However it is recommended that a detailed investigation be undertaken with regard to possibilities for an adjustment of heavy-metal loads while including new measurement series and other riverine areas. In the process the desirability of an additional adjustment regarding the concentration of suspended matter shall also be examined.

Basically, a trend analysis should be undertaken only when data for at least seven years is available. This is true not only when adjusted loads but also non-adjusted loads or mean concentration values are used since the possibility of apparent trends being caused by meteorological cycles cannot be ruled out.

On average, using mean concentration values instead of non-adjusted loads (such as the OSPAR load) makes a certain improvement in trend sensitivity possible as against non-adjusted loads. However at the same time, the use of concentrations to an extent also leads to a deterioration of power so much so that the use of mean concentration values for trend analysis is not advisable.

The current annual load should not be calculated on the basis of the adjusted loads but may continue to be done with the OSPAR formula. However it should be borne in mind that substantial errors of assessment could occur particularly in the case of rivers with a marked seasonality. It is therefore recommended that the method be examined and revised in such a manner – while including the CQ function (as per Method L1 or L2) and the daily runoff series

– that the "actual" annual load, that is to say the quantity of a material discharged from the river into the sea, can be more accurately determined.

Where the seasonality of the runoff is extremely pronounced, a modified sampling concept with higher sampling frequency is recommended during the high-water period and, where necessary, reduced sampling during the low-water period in order to reduce the – to an extent – substantial errors of assessment in load determination and enhance trend sensitivity.

11 Summary

In order to prevent a considerable deterioration in the detectability of time trends in riverine loads as a result of fluctuations in the runoff quantity, an adjustment whereby the entry data are recomputed into an "average" runoff level appears inevitable.

Accordingly, the aim of the project was the development of a concept for the adjustment and trend analysis of riverine loads including the examination of a number of statistical methods, with the form of the load adjustment being the focus of the work. As per this concept, adjustment takes place on the basis of raw data using a dynamically adapted concentration-runoff function. The adjusted loads are then compiled into annual loads before trend analysis follows on the basis of these adjusted annual loads. Finally the trend sensitivity of the method is examined as part of a power analysis.

Nine adjustment methods were tested with seven parameters (NO_3-N, NH_4-N, P_{total}, PO_4-P, Cd, Pb and suspended matter) which were determined once a fortnight in the Rhine at Lobith and once a month in the Ems at Herbrum. In the case of the Rhine, the use of adjusted loads instead of non-adjusted values makes a considerable improvement in trend sensitivity possible for NO_3-N, P_{total} and suspended matter. On the other hand, the use of annual mean concentration values leads to a reduction in trend sensitivity. In the case of the Ems, adjusted loads as well as annual mean concentration values made a higher trend sensitivity possible in every respect as against non-adjusted loads.

In general, the evaluations conducted confirm the practicability of the adjustment concept developed, with no method however appearing optimal for all rivers and substances. A method based on a local regression model with reciprocal runoff rate seems advisable for the adjustment of nutrients and makes a substantial improvement in trend sensitivity possible as compared to the OSPAR load. In the case of the heavy metals examined, the advantages were found to be smaller though it must be assumed that this is at least partly attributable to chemical-analytical problems. The use of more complex regression models may be necessary for the adjustment of heavy metal loads.

A software program was developed as part of the project for carrying out extensive calculations. It was with this software that the various adjustment methods were implemented and tested.

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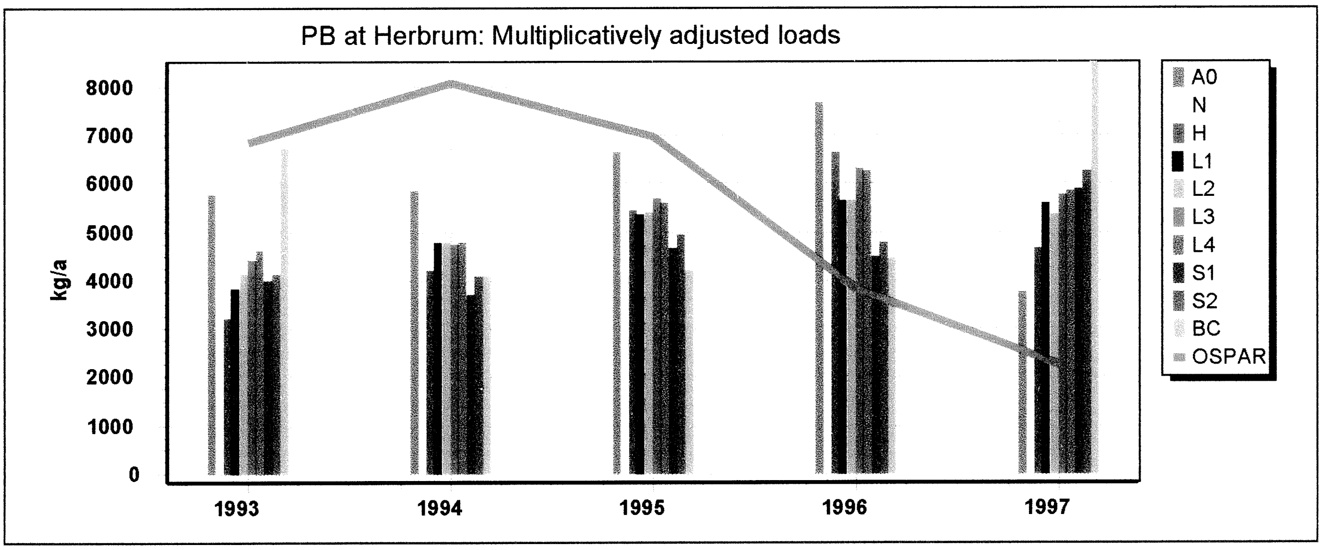
Acknowledgements

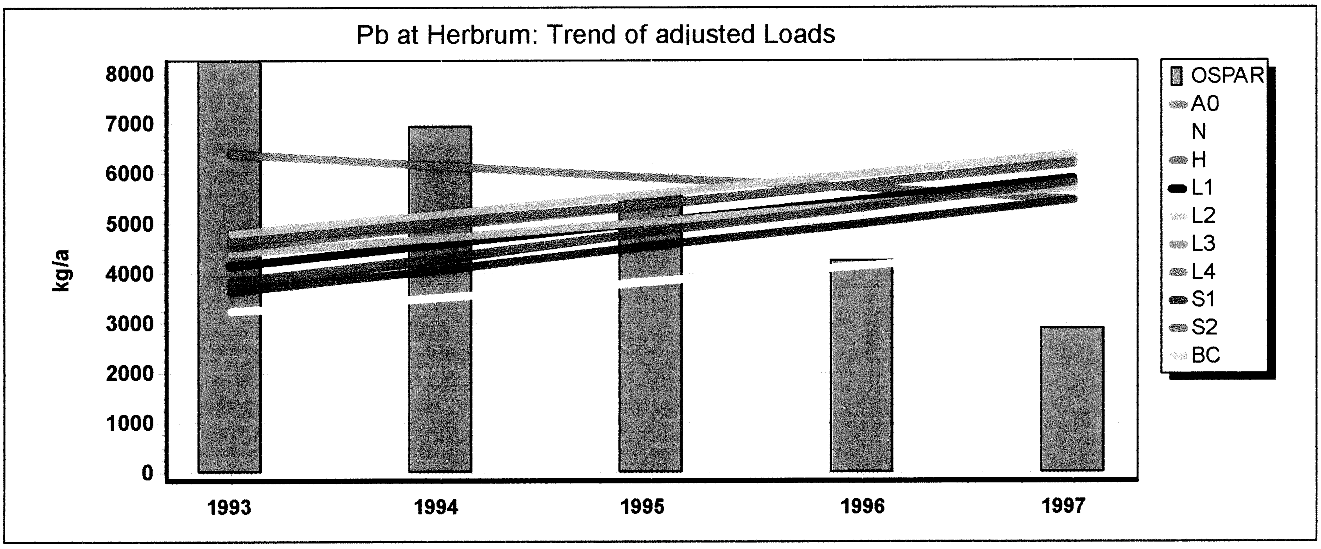
Our special thanks to Dr. Ms. Herata and Mr. Mehlhorn (UBA) for their deep commitment to the research project. We would also like to thank the other members of the working group for their invaluable suggestions and contributions to discussions, with a special word of thanks to Mr. Steffen (NLÖ), Mr. Henneberg (ARGE Weser), Mr. Brunswig (Gewässerschutz Kiel) as well as Mr. Hilden (BfG). We would like to express our gratitude to IGB as well as BfG for making available extensive measurement data for the Rhine, to ARGE Elbe for data for the Elbe and LANU for data for the Trave and the NLÖ for data for the Ems. Numerous discussions held with other known experts have contributed to the project results. Thus discussions with Dr. Stalnacke (Norway) proved extremely useful while preparing the adjustment concept. Prof. Dr. Hebbel (Hamburg University) supported the implementation of the so-called Hebbel Method with his hints. In order to facilitate a comparison between the various methods, Mr. Brunswig conducted a parallel evaluation on the basis of the TRANSPOS load calculation method developed by him.

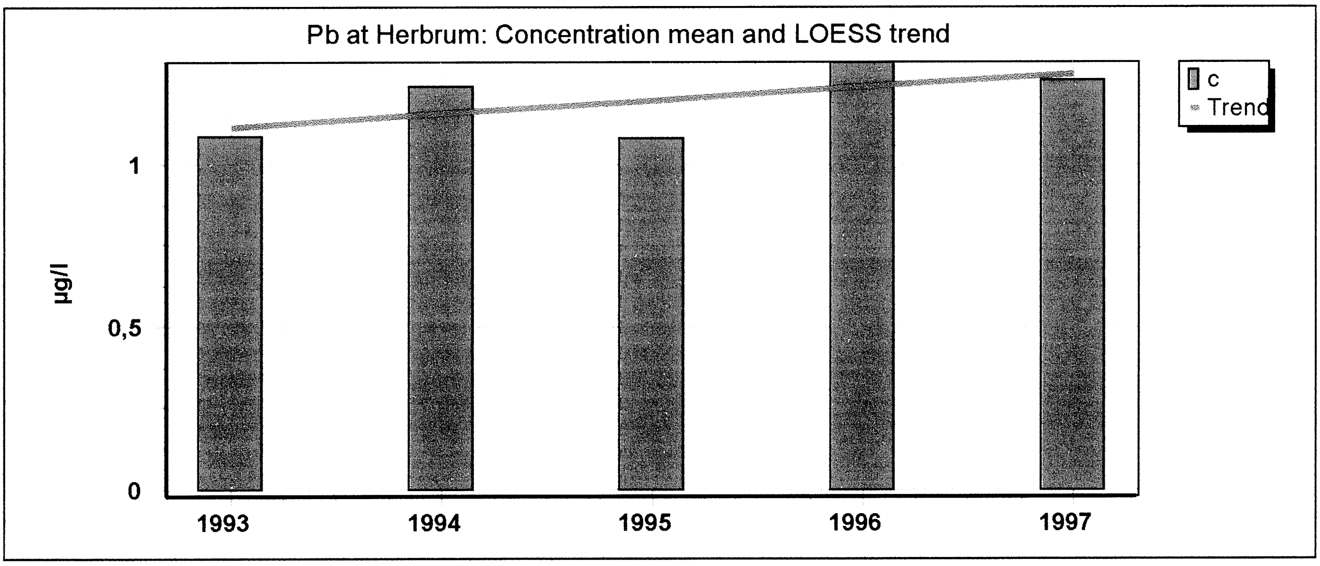
Intensive discussions on adjustment concepts in the ICES working group WGSEM (Working Group on the Statistical Aspects of Environmental Monitoring) have made no insignificant contribution to the development of a sustainable and flexible adjustment concept. Our special thanks in this regard go to Dr. Bjerkeng (NIVA, Oslo) as well as Dr. Fryer (FRS Marine Laboratory, Aberdeen) and Dr. Nicholson (MAFF, Fisheries Laboratories, London).

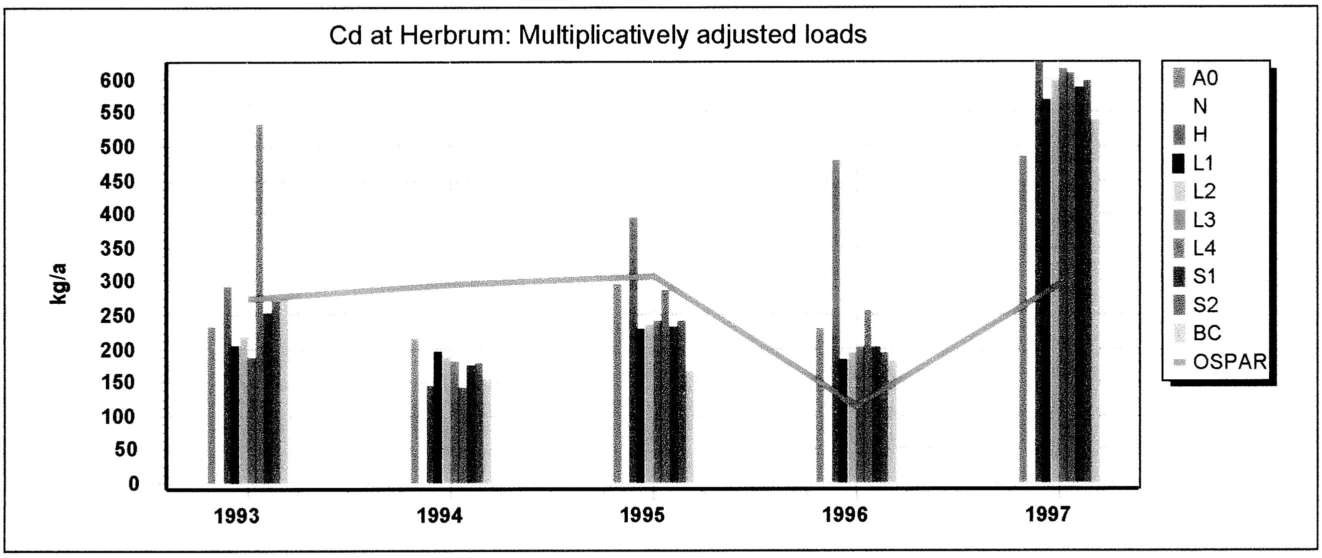
Annex A

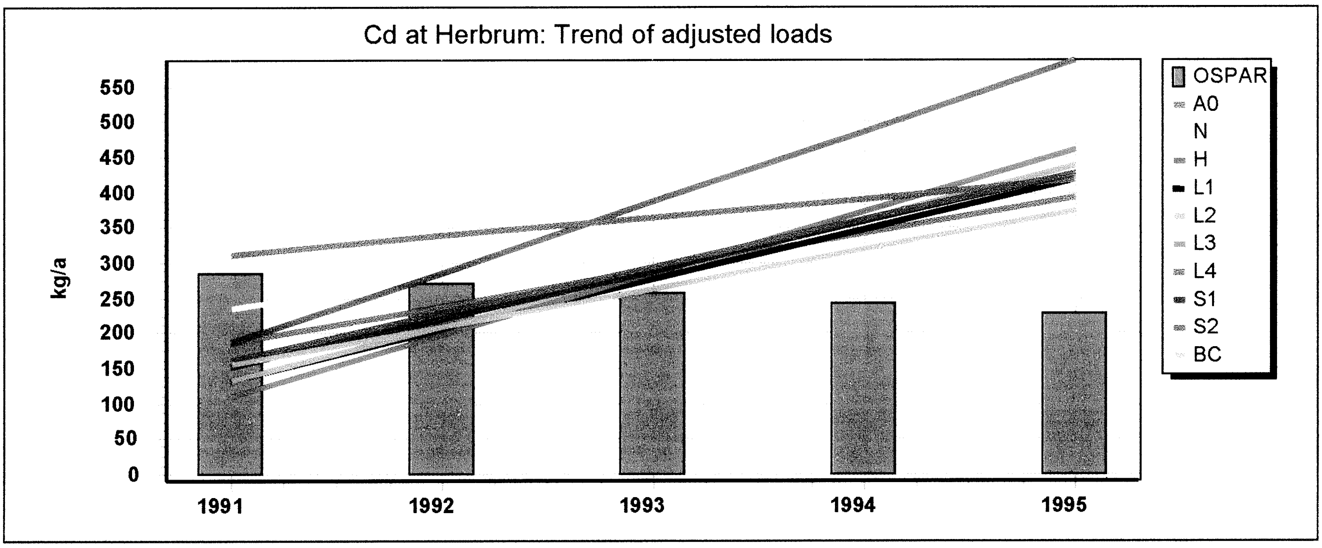
Loads and concentrations for the parameters P_{total}, PO_4-P, NH_4-N, NO_3-N and Suspended matter for the River Ems (Herbrum) and the River Rhine (Lobith).

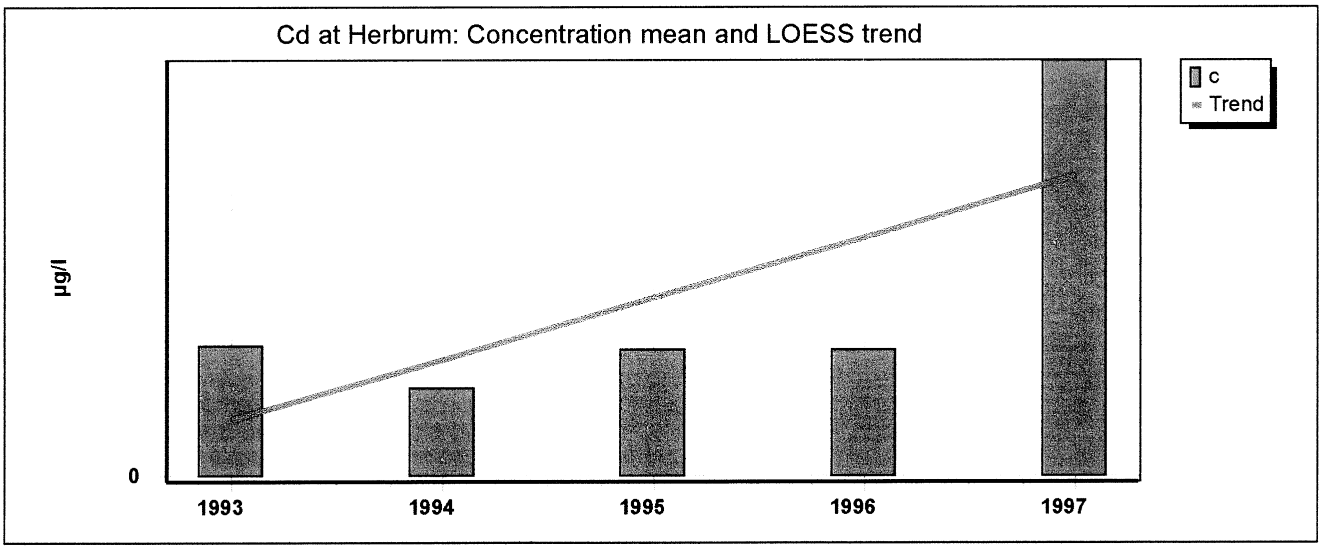

PB at Herbrum: Multiplicatively adjusted loads
kg/a
8000
7000
6000
5000
4000
3000
2000
1000
0
1993
1994
1995
1996
1997
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR

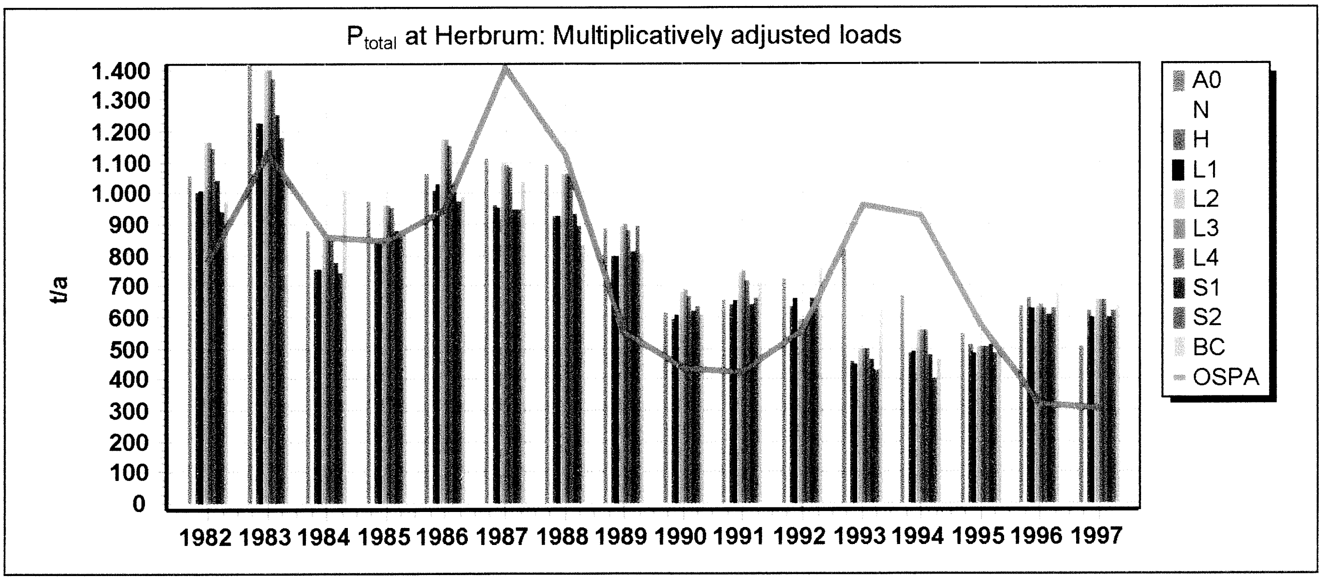

Pb at Herbrum: Trend of adjusted Loads
kg/a
8000
7000
6000
5000
4000
3000
2000
1000
0
1993
1994
1995
1996
1997
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC

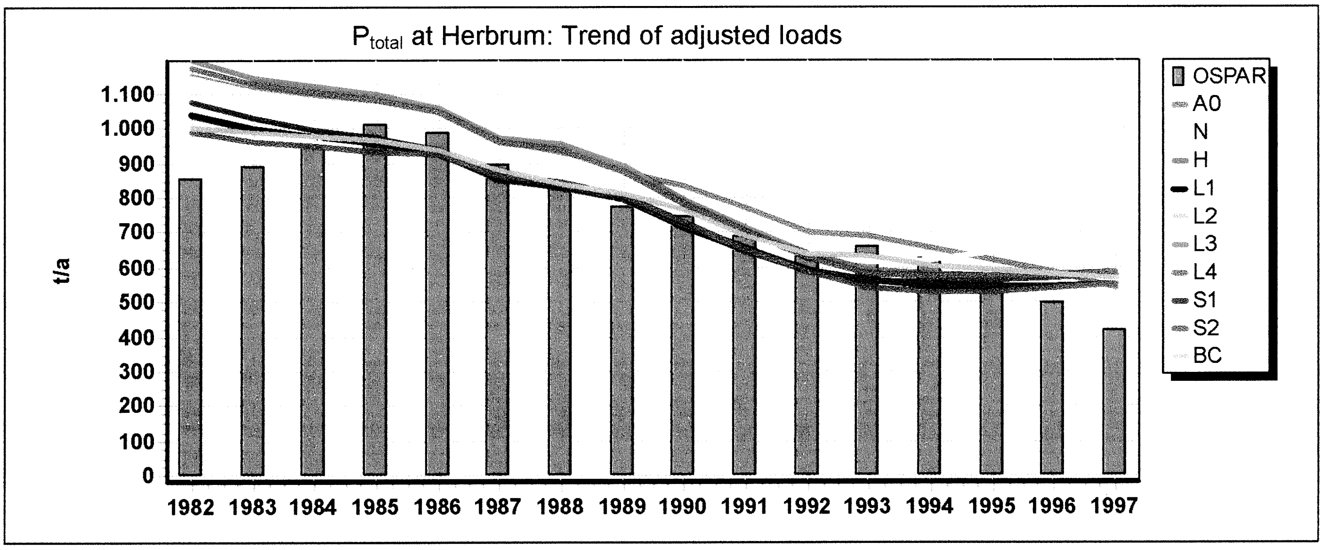

Pb at Herbrum: Concentration mean and LOESS trend
µg/l
1
0,5
0
1993
1994
1995
1996
1997
c
Trend

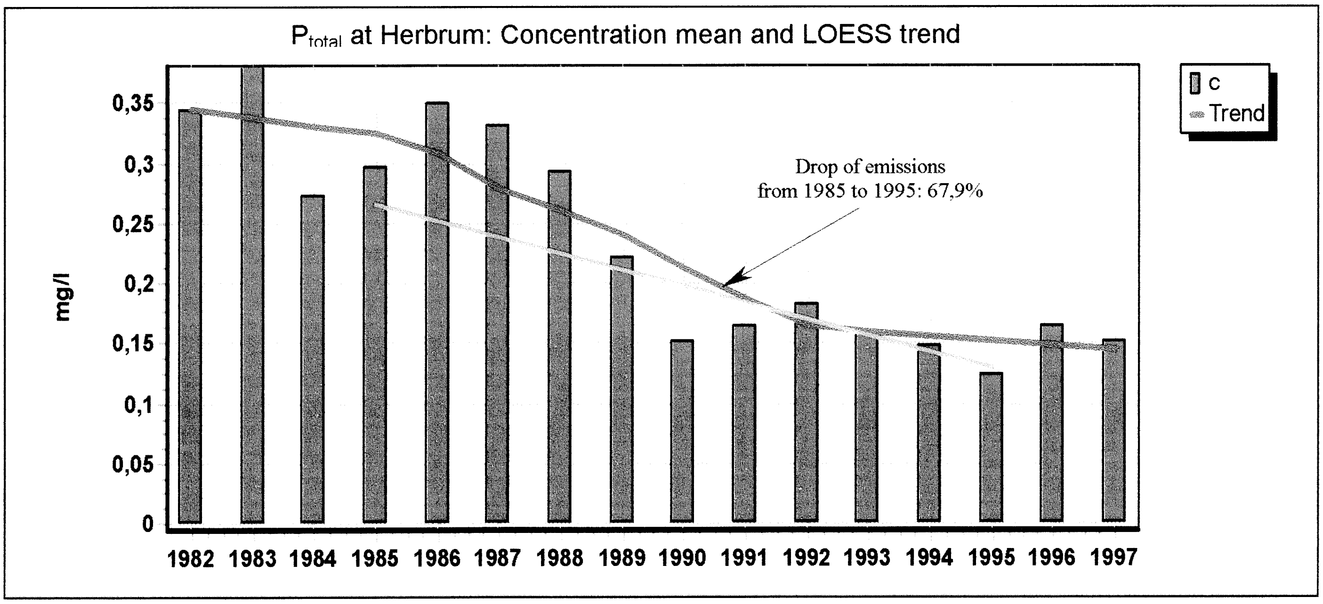

Cd at Herbrum: Multiplicatively adjusted loads
kg/a
600
550
500
450
400
350
300
250
200
150
100
50
0
1993
1994
1995
1996
1997
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR

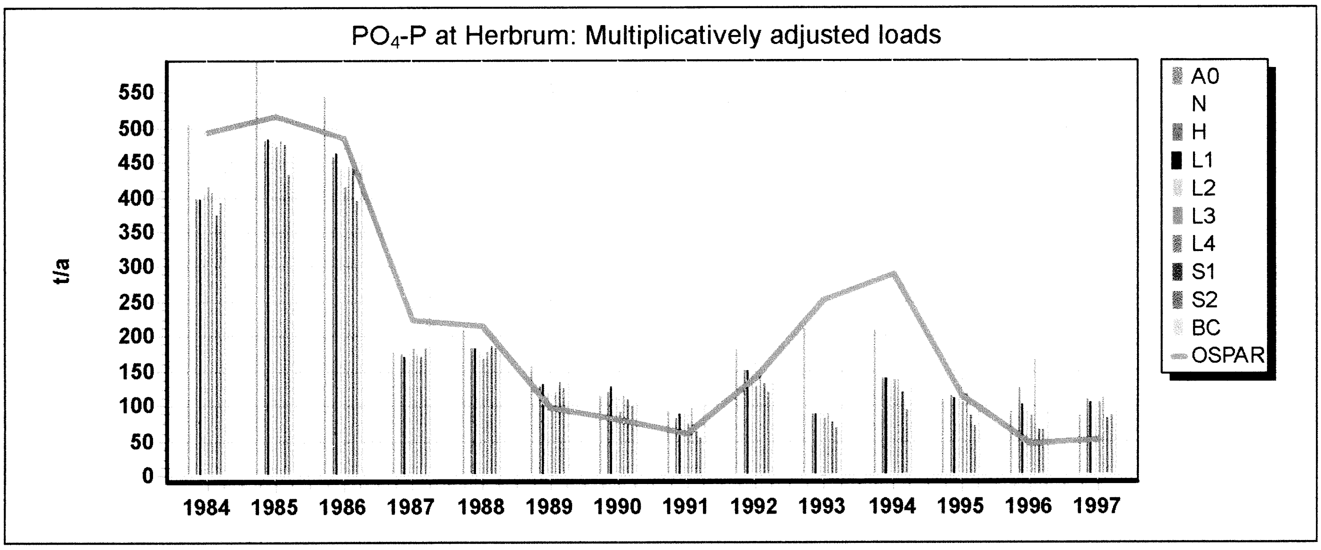

Cd at Herbrum: Trend of adjusted loads
kg/a
550
500
450
400
350
300
250
200
150
100
50
0
1991
1992
1993
1994
1995
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC


Cd at Herbrum: Concentration mean and LOESS trend
µg/l
0
1993
1994
1995
1996
1997
c
Trend

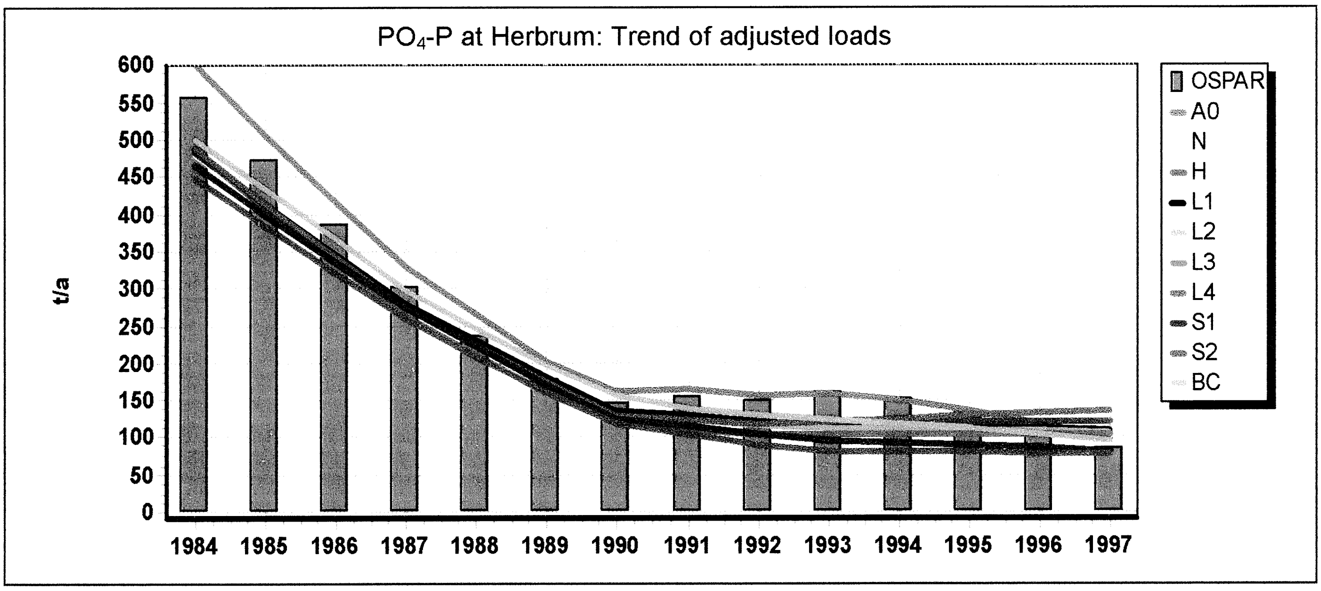

P_{total} at Herbrum: Multiplicatively adjusted loads
t/a
1.400
1.300
1.200
1.100
1.000
900
800
700
600
500
400
300
200
100
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPA


P_{total} at Herbrum: Trend of adjusted loads
t/a
1.100
1.000
900
800
700
600
500
400
300
200
100
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC

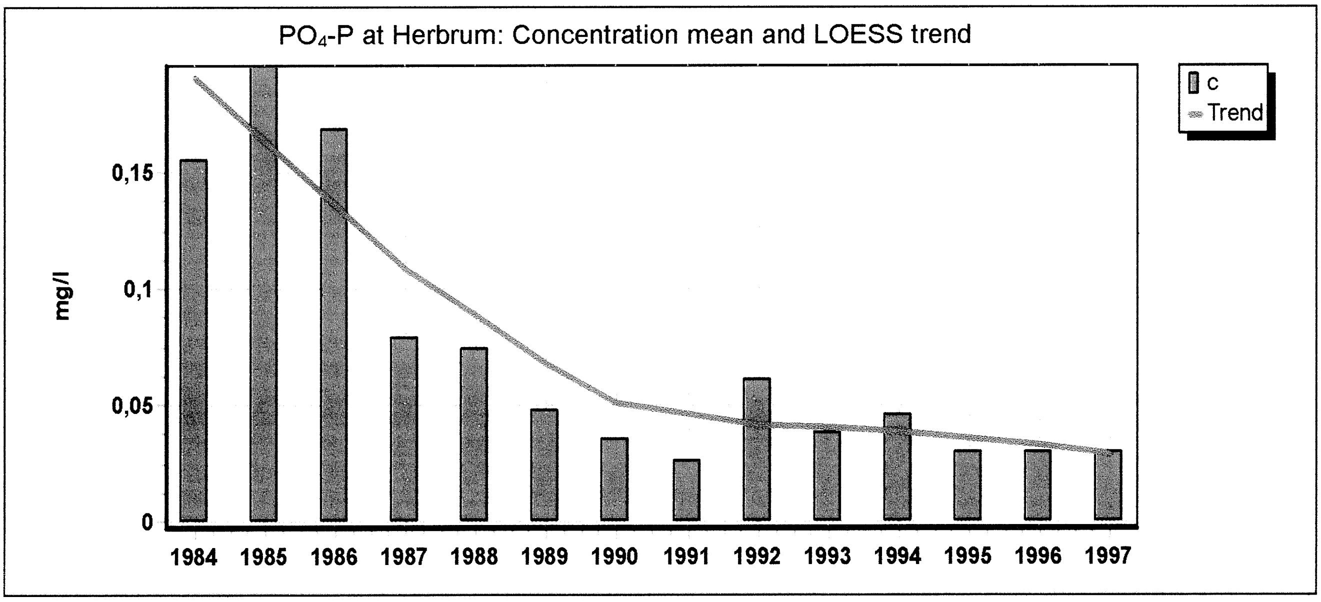

P_{total} at Herbrum: Concentration mean and LOESS trend
mg/l
0,35
0,3
0,25
0,2
0,15
0,1
0,05
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
c
Trend
Drop of emissions
from 1985 to 1995: 67,9%



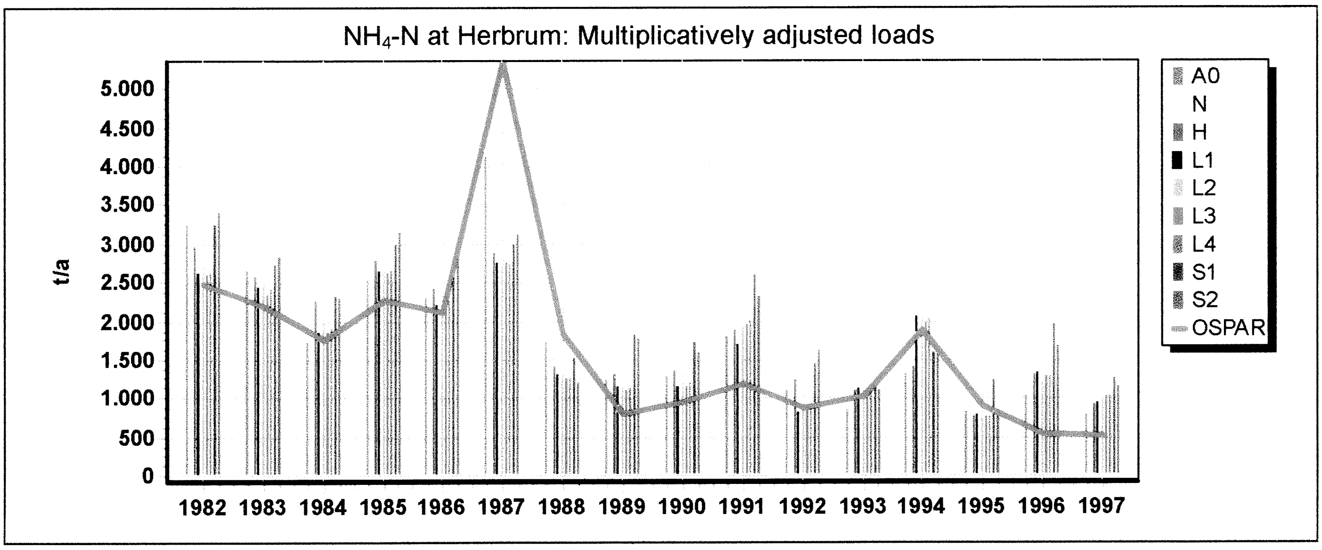
PO4-P at Herbrum: Multiplicatively adjusted loads
t/a
550
500
450
400
350
300
250
200
150
100
50
0
1984
1985
1986
1987
1988
1989
1990
1991
1992
1993
1994
1995
1996
1997
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR

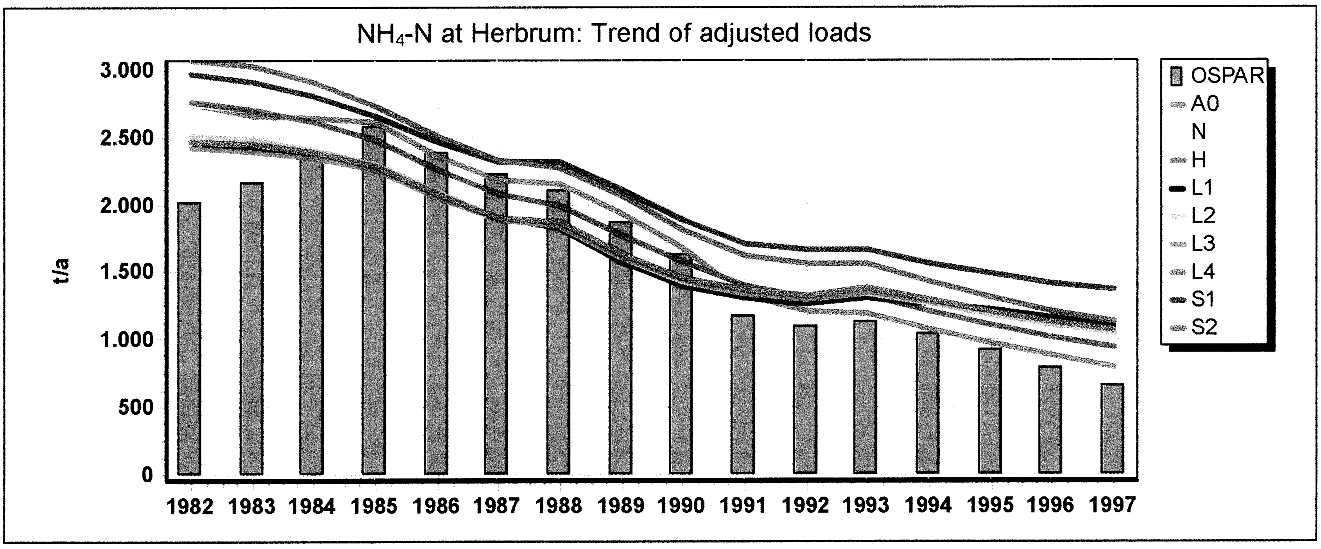


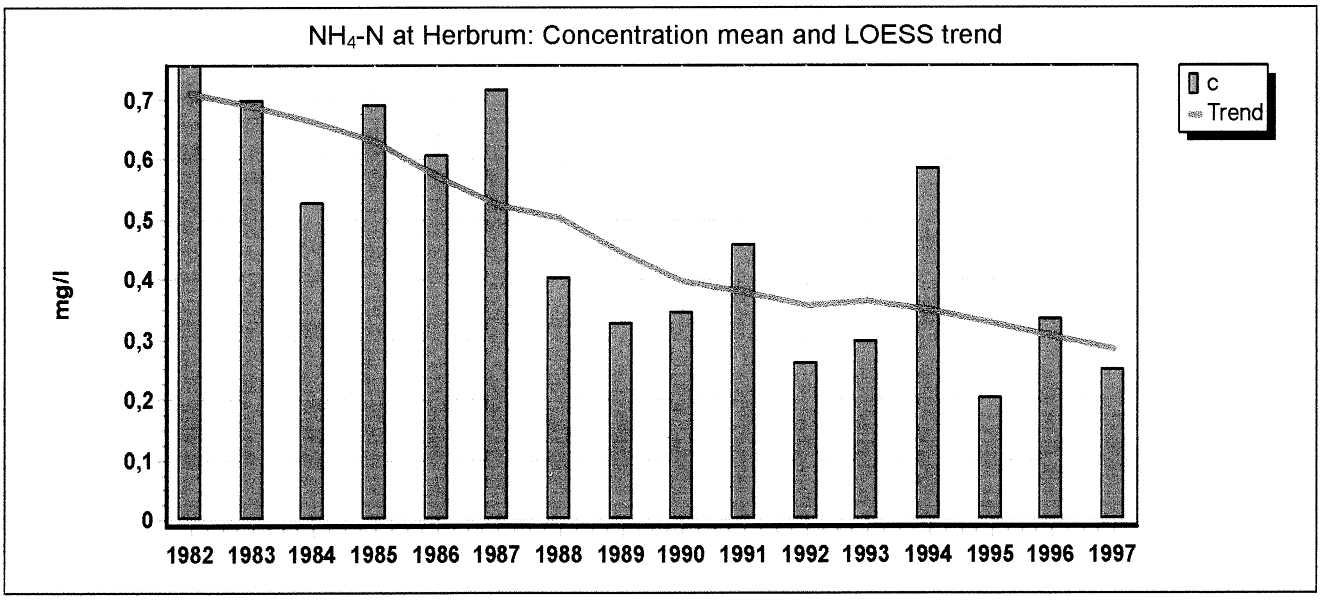
PO4-P at Herbrum: Trend of adjusted loads
t/a
600
550
500
450
400
350
300
250
200
150
100
50
0
1984
1985
1986
1987
1988
1989
1990
1991
1992
1993
1994
1995
1996
1997
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC

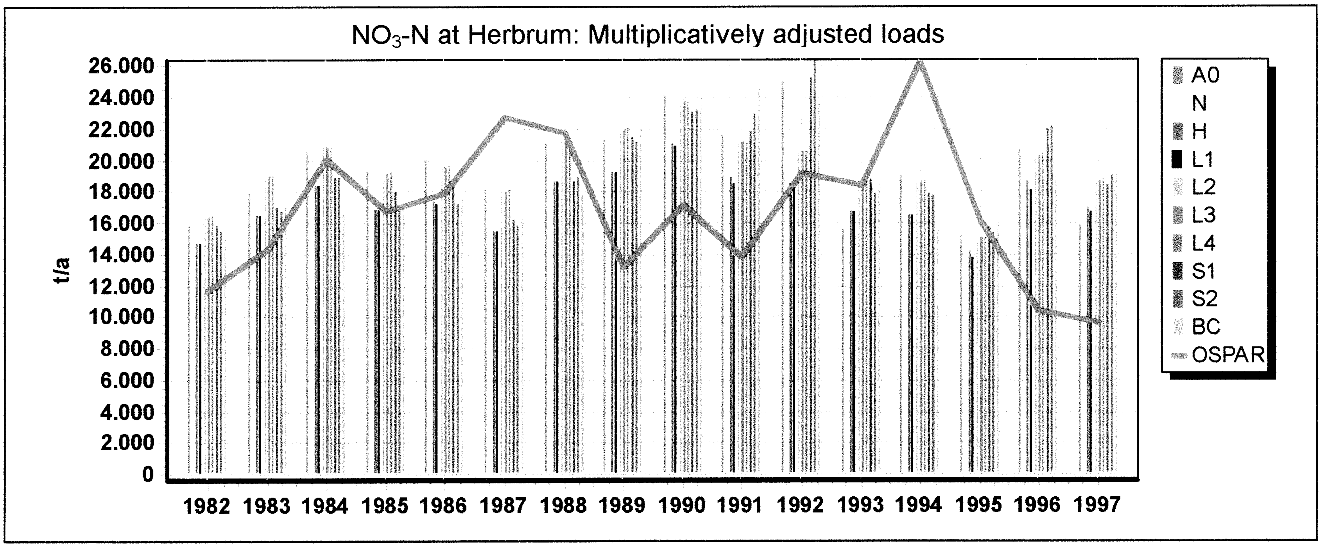


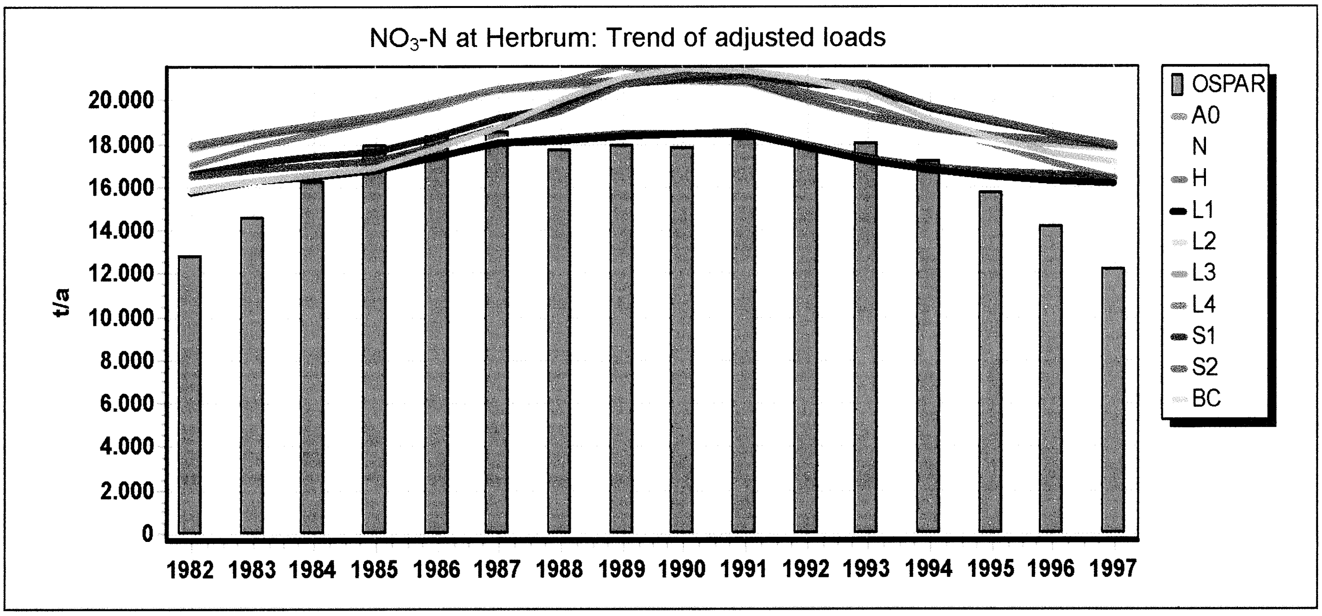
PO4-P at Herbrum: Concentration mean and LOESS trend
mg/l
0,15
0,1
0,05
0
1984
1985
1986
1987
1988
1989
1990
1991
1992
1993
1994
1995
1996
1997
c
Trend

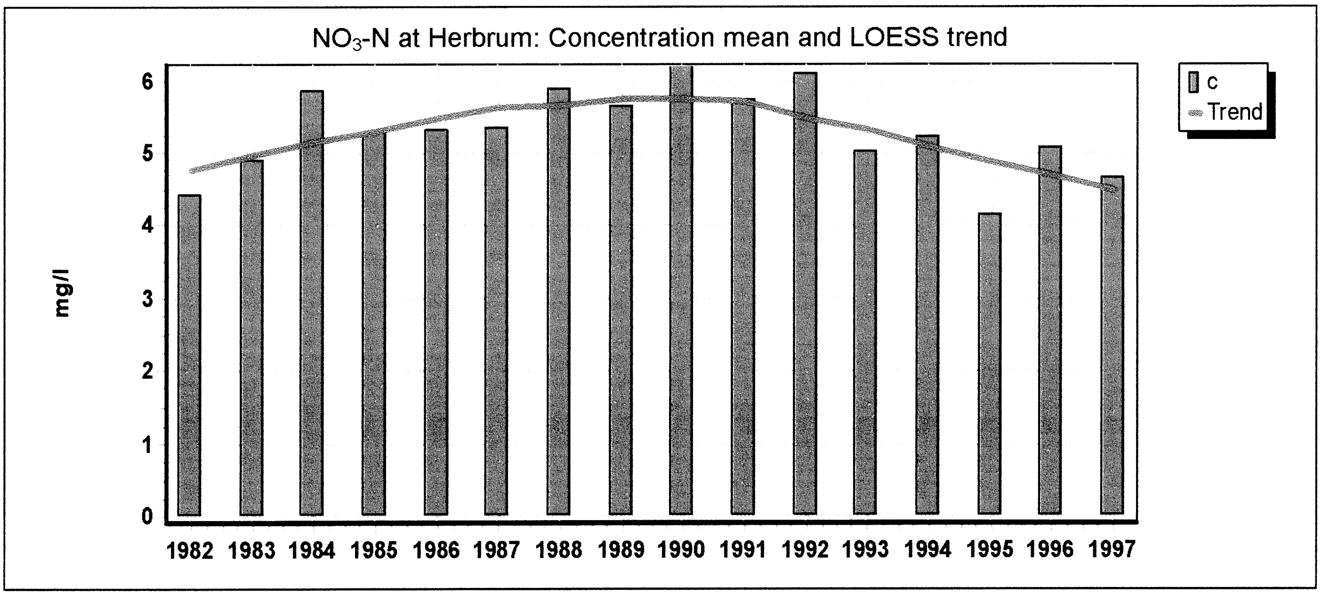

NH4-N at Herbrum: Multiplicatively adjusted loads
t/a
5.000
4.500
4.000
3.500
3.000
2.500
2.000
1.500
1.000
500
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
A0
N
H
L1
L2
L3
L4
S1
S2
OSPAR

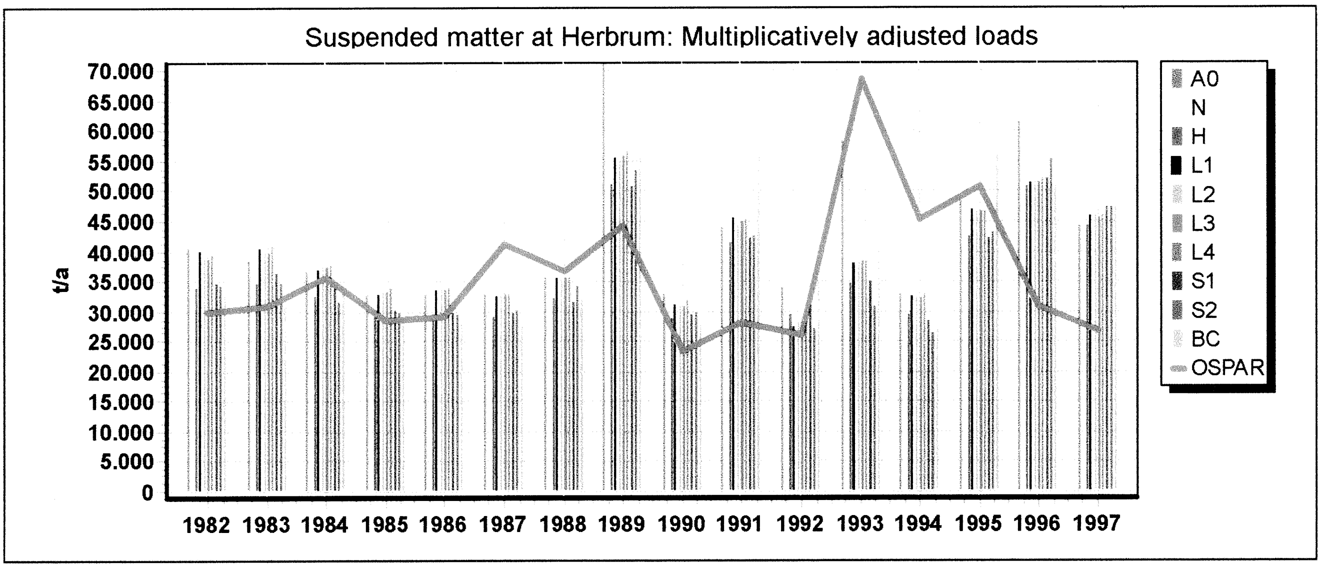

NH4-N at Herbrum: Trend of adjusted loads
t/a
3.000
2.500
2.000
1.500
1.000
500
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2

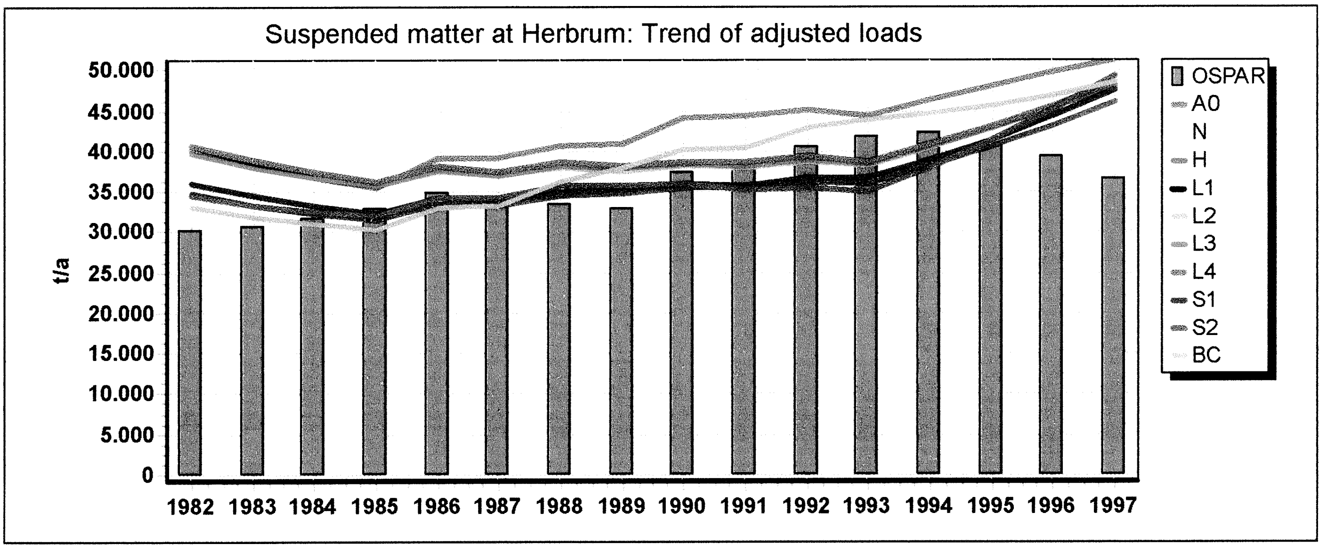

NH4-N at Herbrum: Concentration mean and LOESS trend
mg/l
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
c
Trend

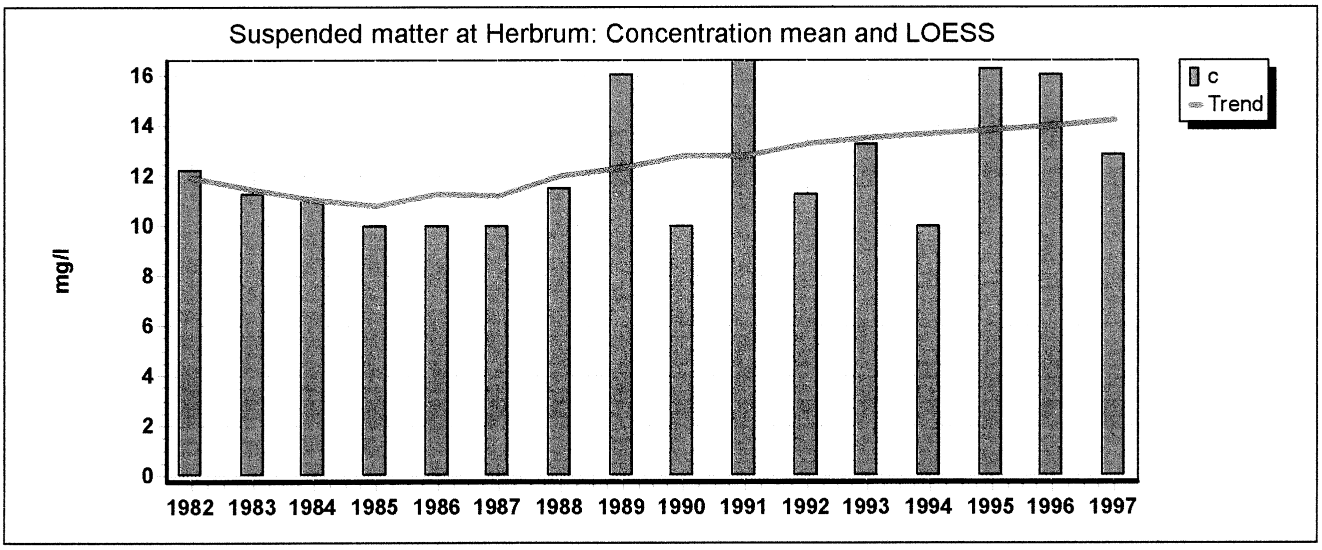

NO3-N at Herbrum: Multiplicatively adjusted loads
t/a
26.000
24.000
22.000
20.000
18.000
16.000
14.000
12.000
10.000
8.000
6.000
4.000
2.000
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR

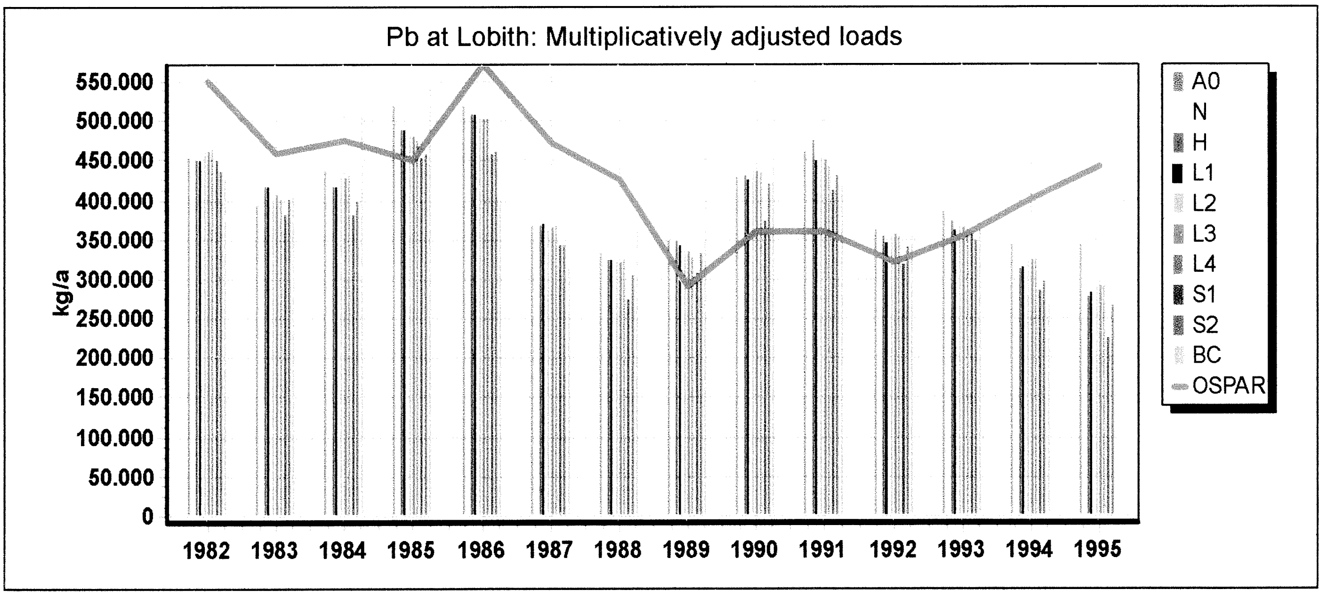

NO3-N at Herbrum: Trend of adjusted loads
t/a
20.000
18.000
16.000
14.000
12.000
10.000
8.000
6.000
4.000
2.000
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC

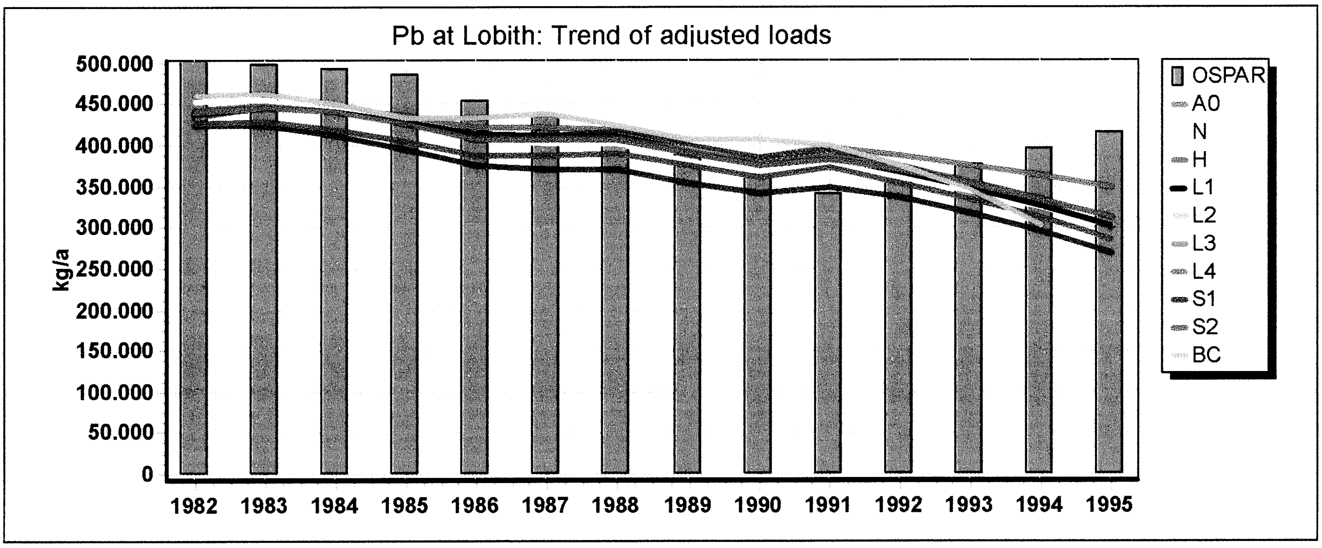

NO3-N at Herbrum: Concentration mean and LOESS trend
mg/l
6
5
4
3
2
1
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
c
Trend

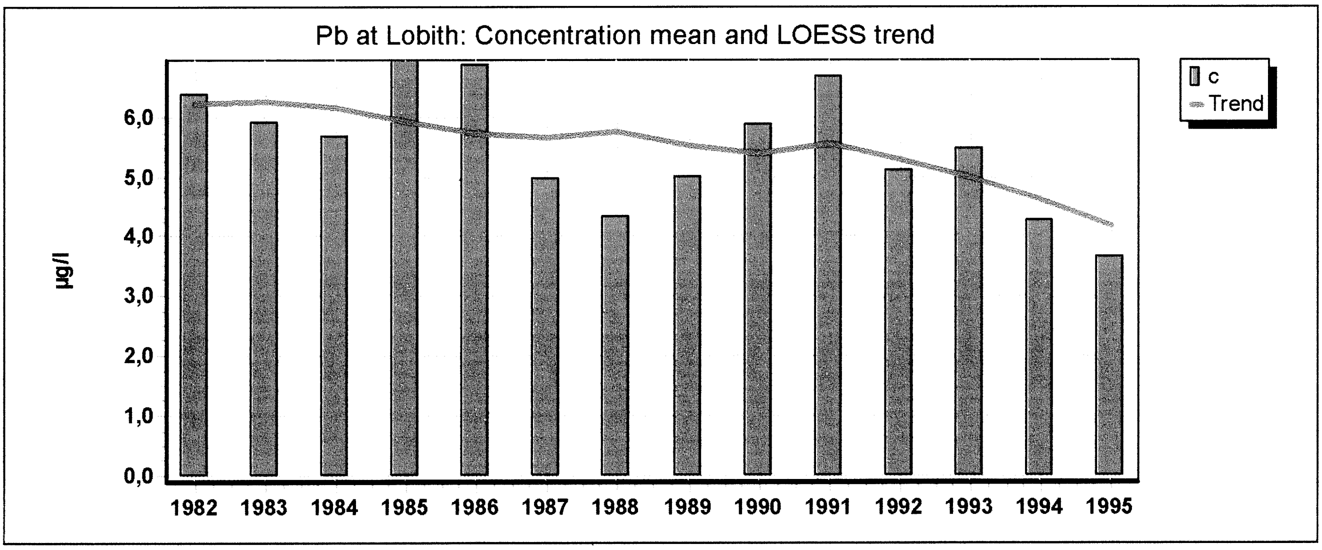

Suspended matter at Herbrum: Multiplicatively adjusted loads
t/a
70.000
65.000
60.000
55.000
50.000
45.000
40.000
35.000
30.000
25.000
20.000
15.000
10.000
5.000
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR

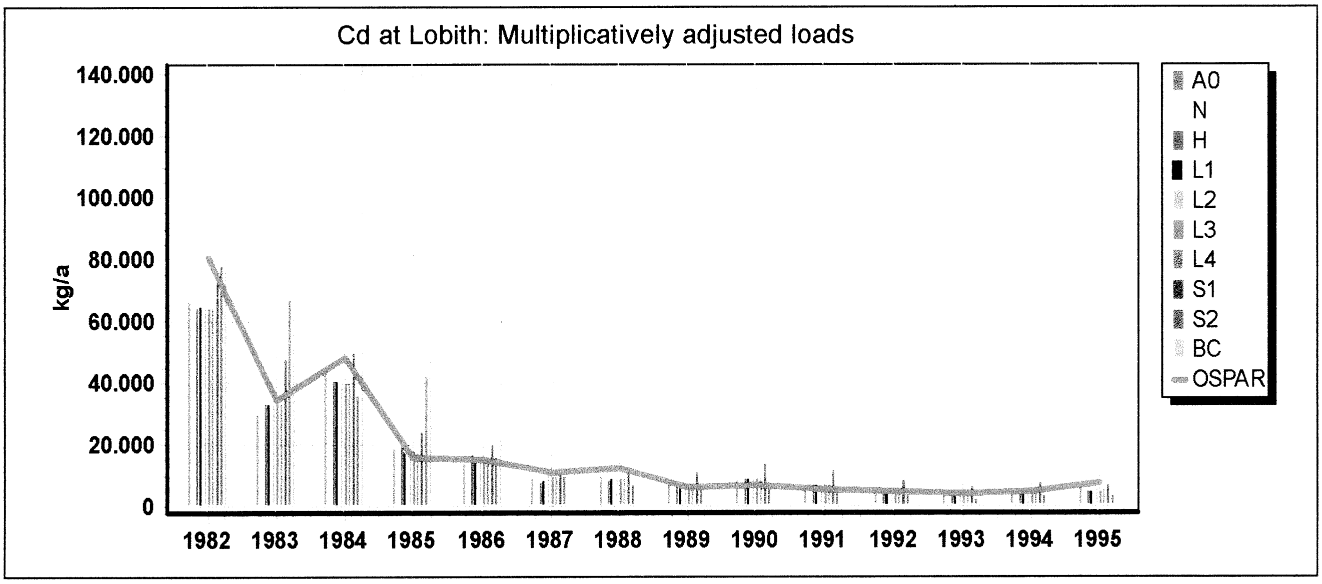

Suspended matter at Herbrum: Trend of adjusted loads
t/a
50.000
45.000
40.000
35.000
30.000
25.000
20.000
15.000
10.000
5.000
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC

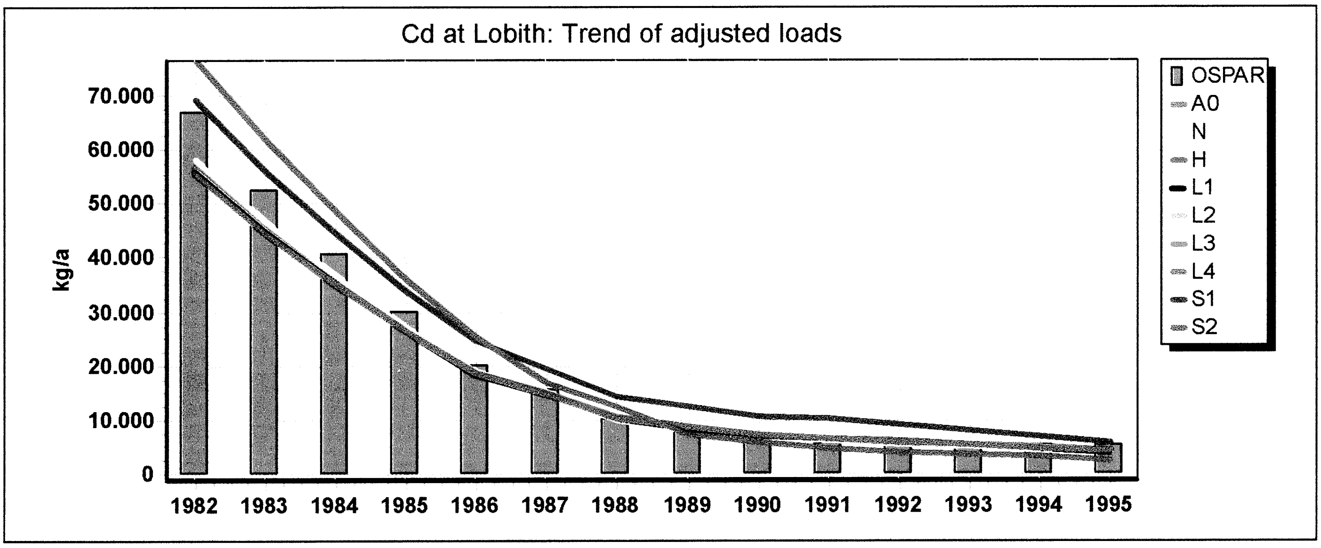

Suspended matter at Herbrum: Concentration mean and LOESS
mg/l
16
14
12
10
8
6
4
2
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997
c
Trend

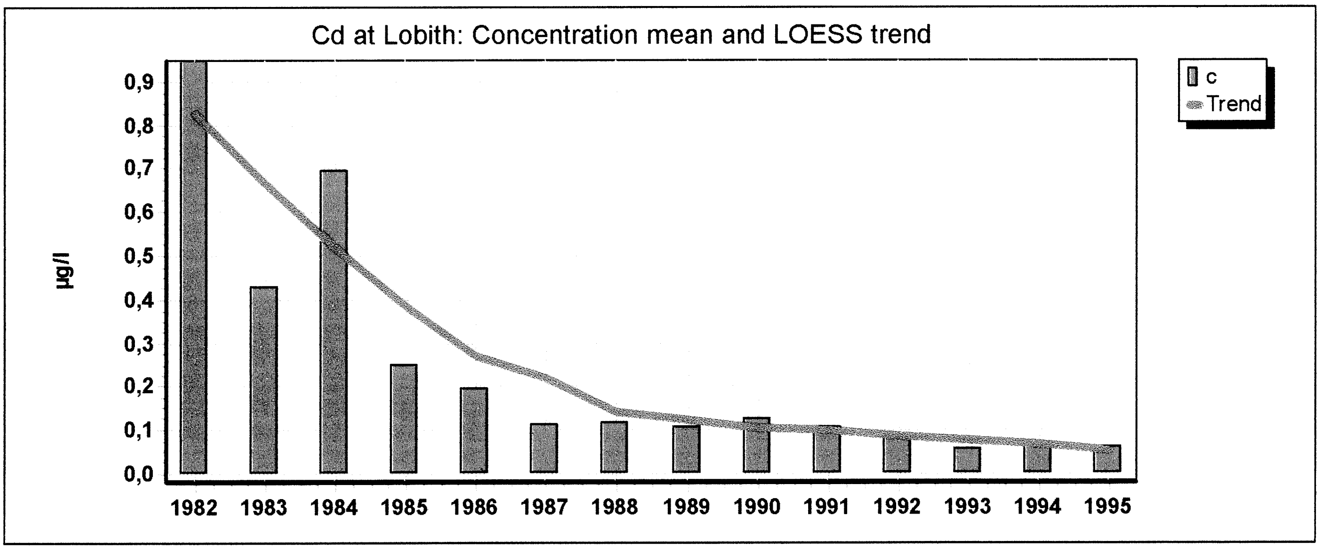

Pb at Lobith: Multiplicatively adjusted loads
550.000
500.000
450.000
400.000
350.000
300.000
250.000
200.000
150.000
100.000
50.000
0
kg/a
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR

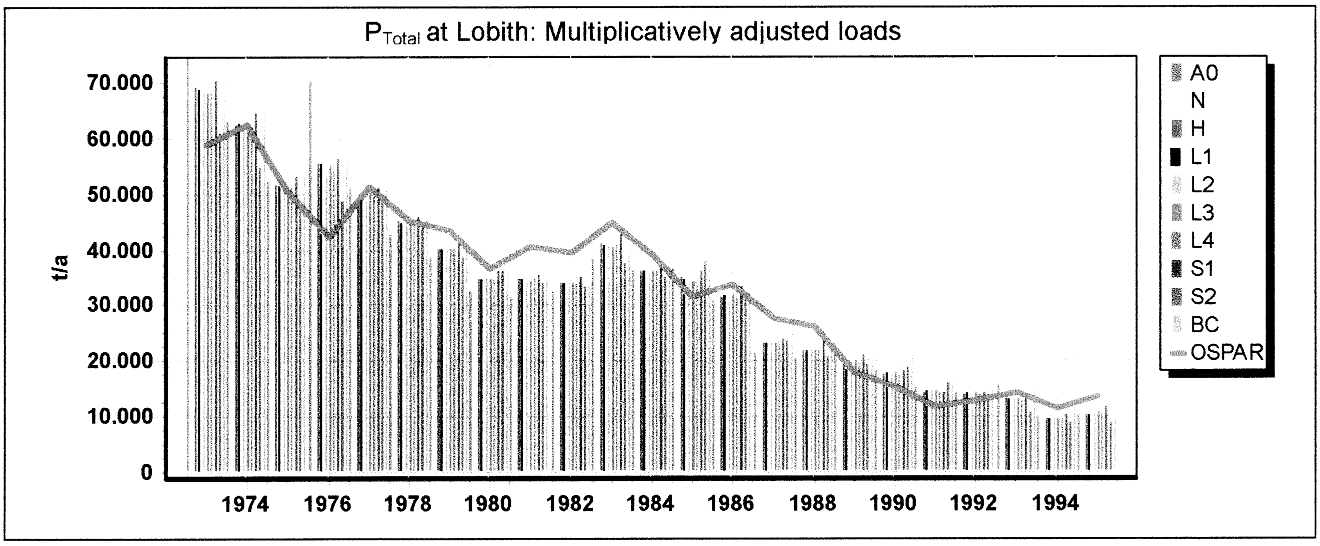

Pb at Lobith: Trend of adjusted loads
500.000
450.000
400.000
350.000
300.000
250.000
200.000
150.000
100.000
50.000
0
kg/a
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC


Pb at Lobith: Concentration mean and LOESS trend
6,0
5,0
4,0
3,0
2,0
1,0
0,0
µg/l
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995
c
Trend

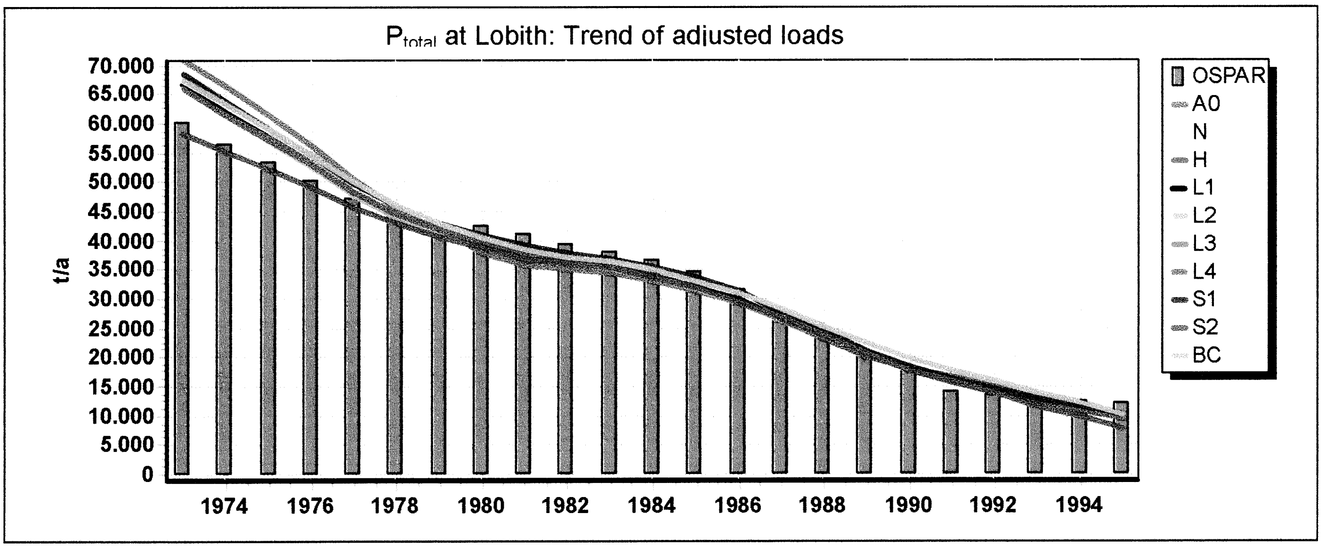

Cd at Lobith: Multiplicatively adjusted loads
kg/a
140.000
120.000
100.000
80.000
60.000
40.000
20.000
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR


Cd at Lobith: Trend of adjusted loads
kg/a
70.000
60.000
50.000
40.000
30.000
20.000
10.000
0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2

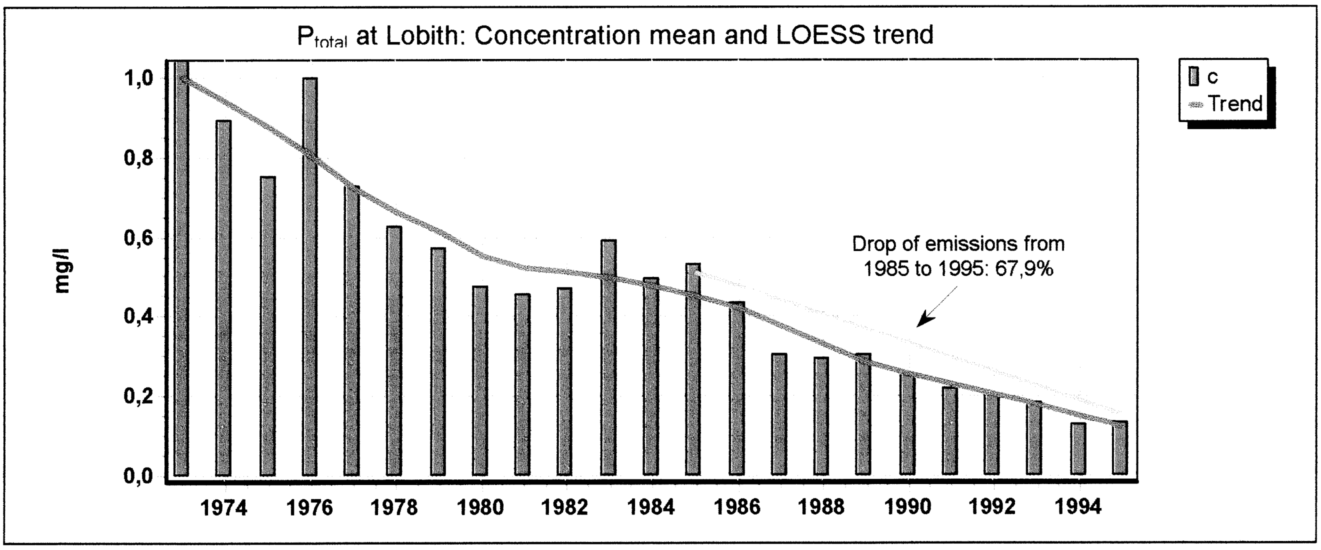

Cd at Lobith: Concentration mean and LOESS trend
µg/l
0,9
0,8
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0,0
1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995
c
Trend



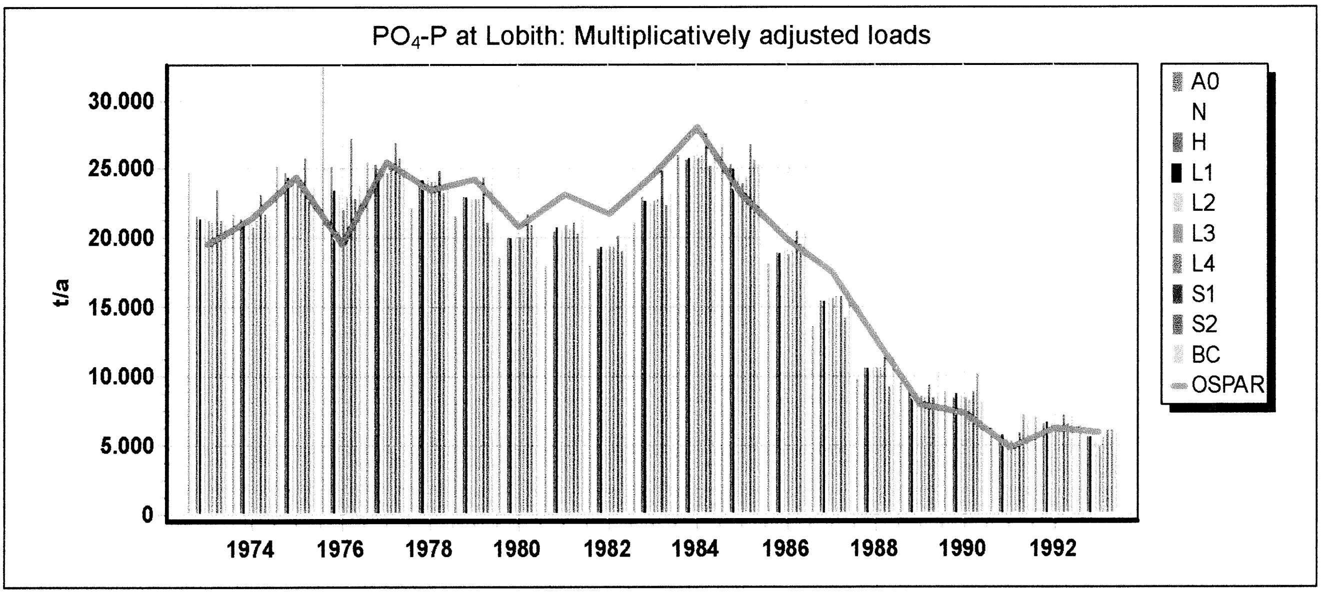
P_{Total} at Lobith: Multiplicatively adjusted loads
t/a
70.000
60.000
50.000
40.000
30.000
20.000
10.000
0
1974
1976
1978
1980
1982
1984
1986
1988
1990
1992
1994
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR

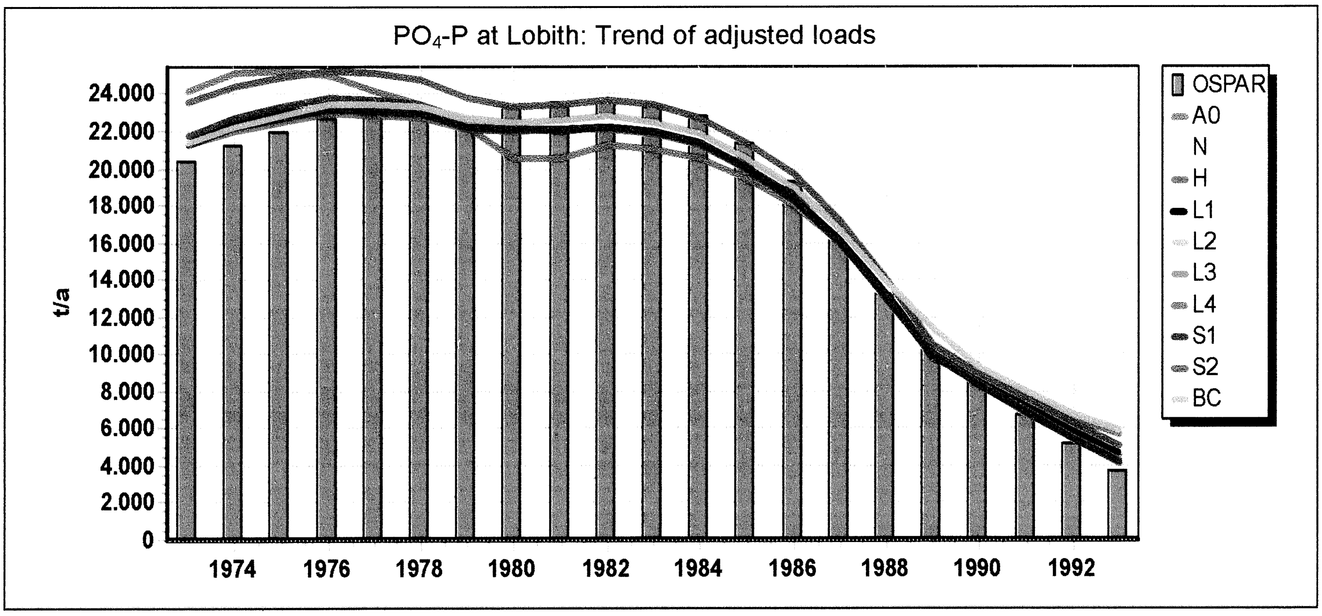


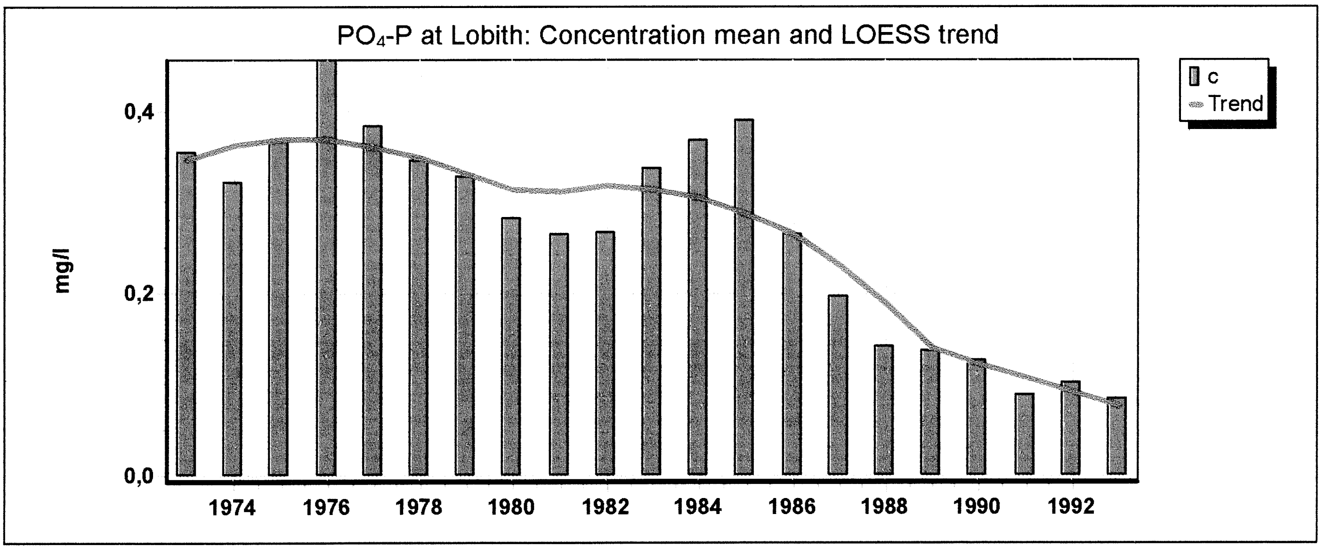
P_{total} at Lobith: Trend of adjusted loads
t/a
70.000
65.000
60.000
55.000
50.000
45.000
40.000
35.000
30.000
25.000
20.000
15.000
10.000
5.000
0
1974
1976
1978
1980
1982
1984
1986
1988
1990
1992
1994
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC

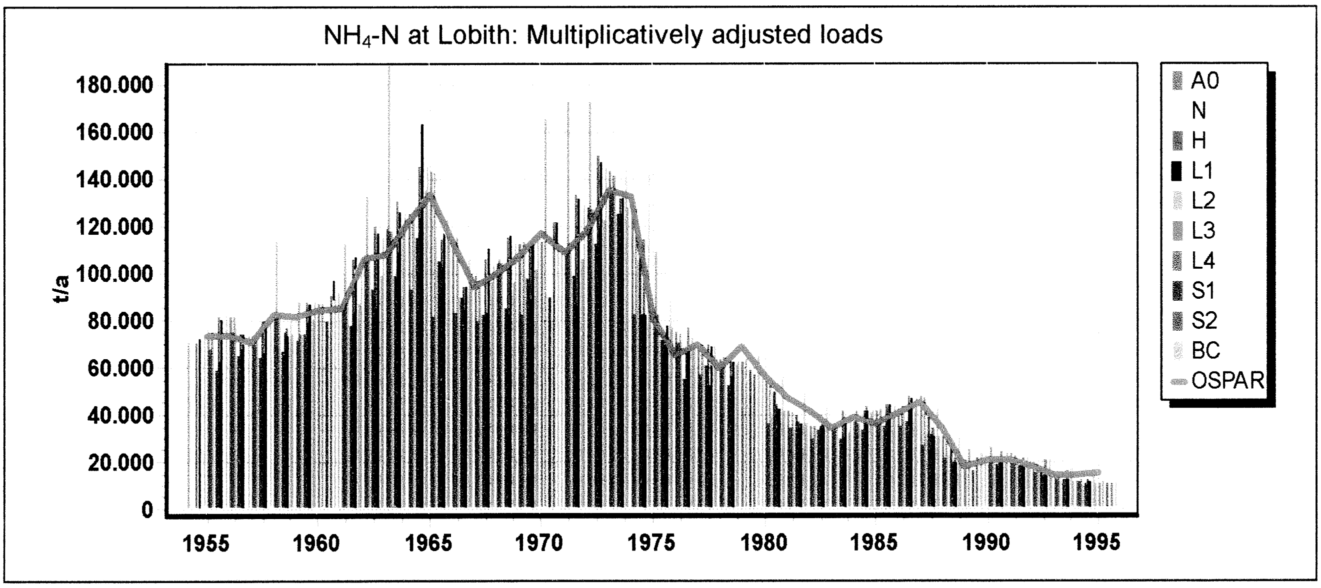


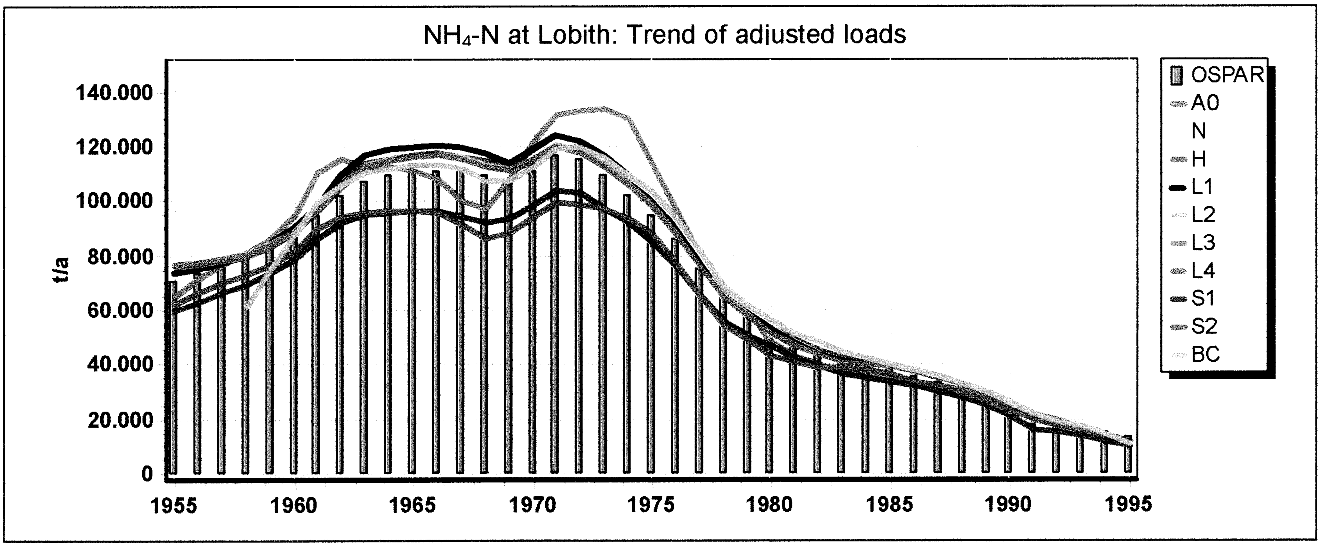
P_{total} at Lobith: Concentration mean and LOESS trend
mg/l
1,0
0,8
0,6
0,4
0,2
0,0
1974
1976
1978
1980
1982
1984
1986
1988
1990
1992
1994
c
Trend
Drop of emissions from 1985 to 1995: 67,9%

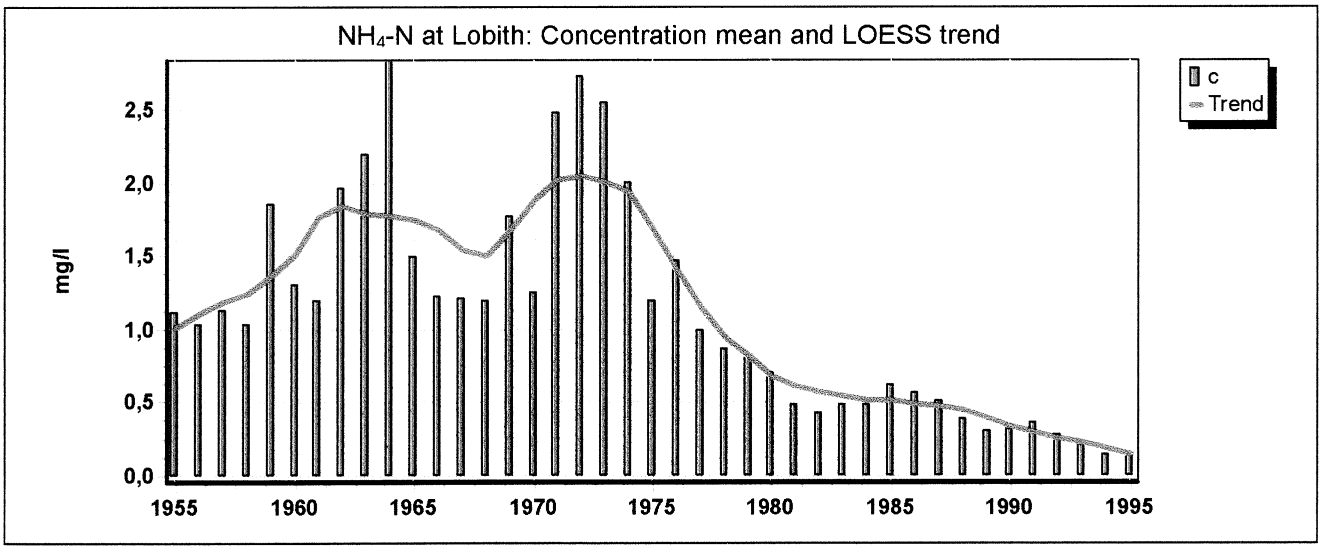

PO4-P at Lobith: Multiplicatively adjusted loads
t/a
30.000
25.000
20.000
15.000
10.000
5.000
0
1974
1976
1978
1980
1982
1984
1986
1988
1990
1992
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR

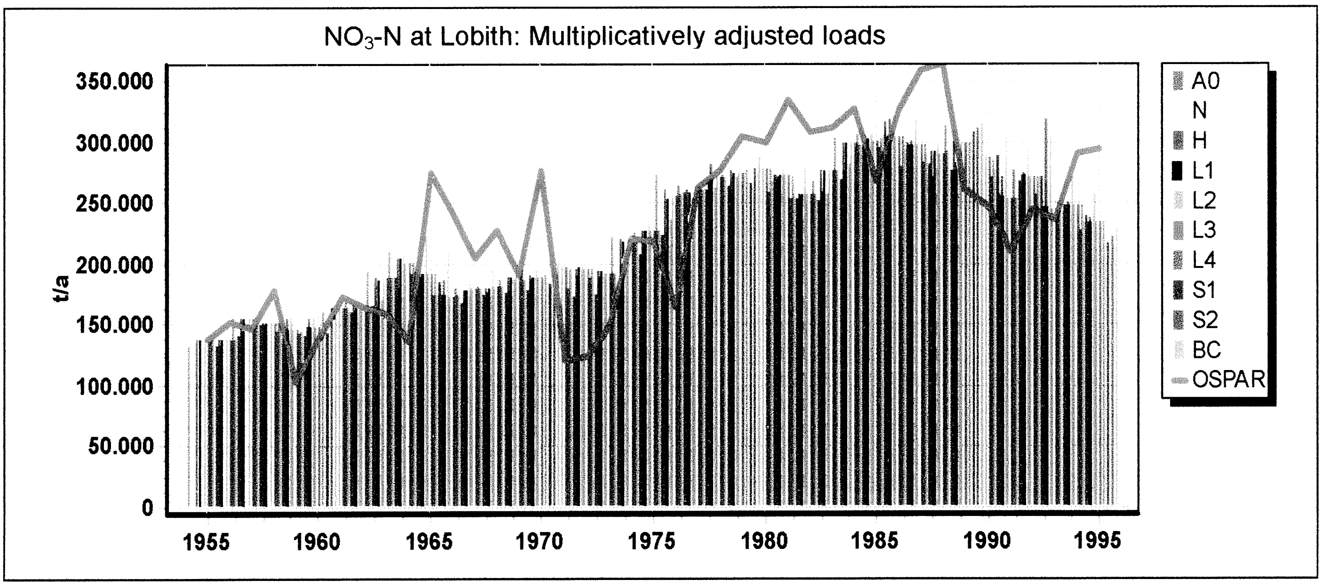

PO4-P at Lobith: Trend of adjusted loads
t/a
24.000
22.000
20.000
18.000
16.000
14.000
12.000
10.000
8.000
6.000
4.000
2.000
0
1974
1976
1978
1980
1982
1984
1986
1988
1990
1992
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC

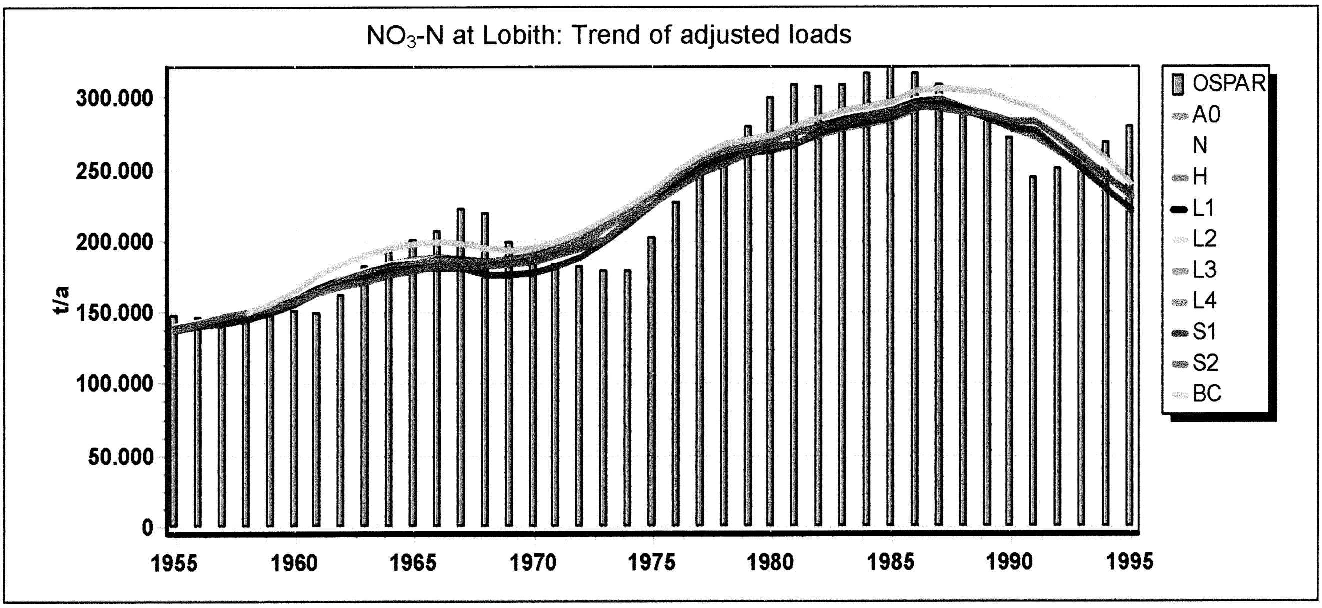

PO4-P at Lobith: Concentration mean and LOESS trend
mg/l
0,4
0,2
0,0
1974
1976
1978
1980
1982
1984
1986
1988
1990
1992
c
Trend

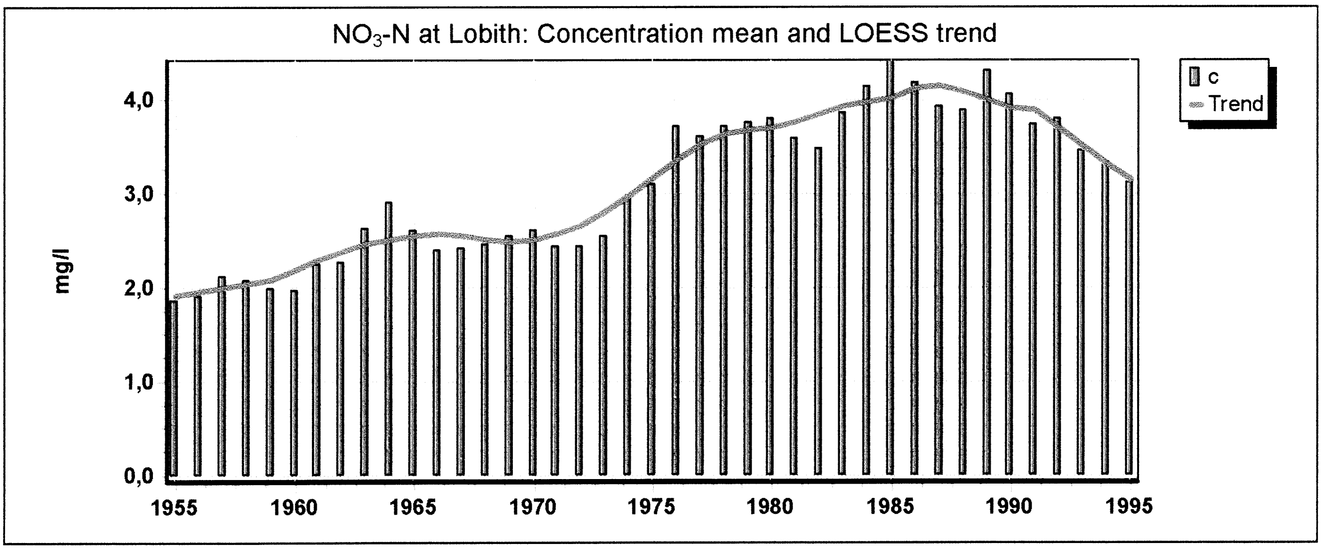

NH4-N at Lobith: Multiplicatively adjusted loads
t/a
180.000
160.000
140.000
120.000
100.000
80.000
60.000
40.000
20.000
0
1955
1960
1965
1970
1975
1980
1985
1990
1995
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR

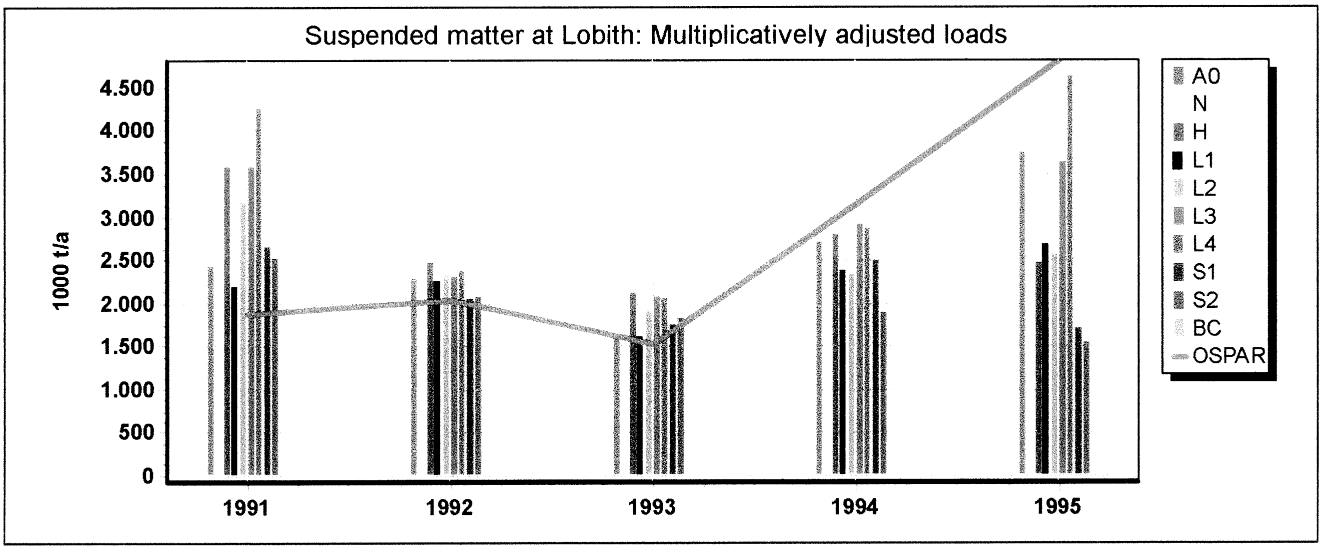

NH4-N at Lobith: Trend of adjusted loads
t/a
140.000
120.000
100.000
80.000
60.000
40.000
20.000
0
1955
1960
1965
1970
1975
1980
1985
1990
1995
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC


NH4-N at Lobith: Concentration mean and LOESS trend
mg/l
2,5
2,0
1,5
1,0
0,5
0,0
1955
1960
1965
1970
1975
1980
1985
1990
1995
c
Trend

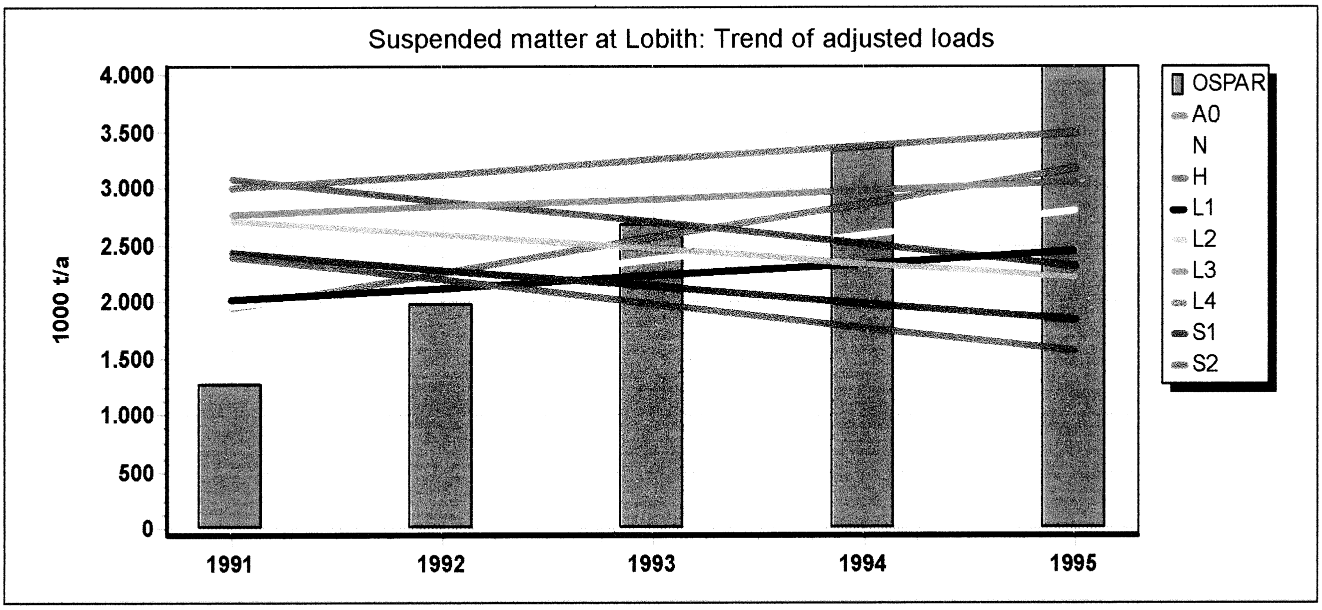

NO3-N at Lobith: Multiplicatively adjusted loads
t/a
350.000
300.000
250.000
200.000
150.000
100.000
50.000
0
1955
1960
1965
1970
1975
1980
1985
1990
1995
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR


NO3-N at Lobith: Trend of adjusted loads
t/a
300.000
250.000
200.000
150.000
100.000
50.000
0
1955
1960
1965
1970
1975
1980
1985
1990
1995
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2
BC

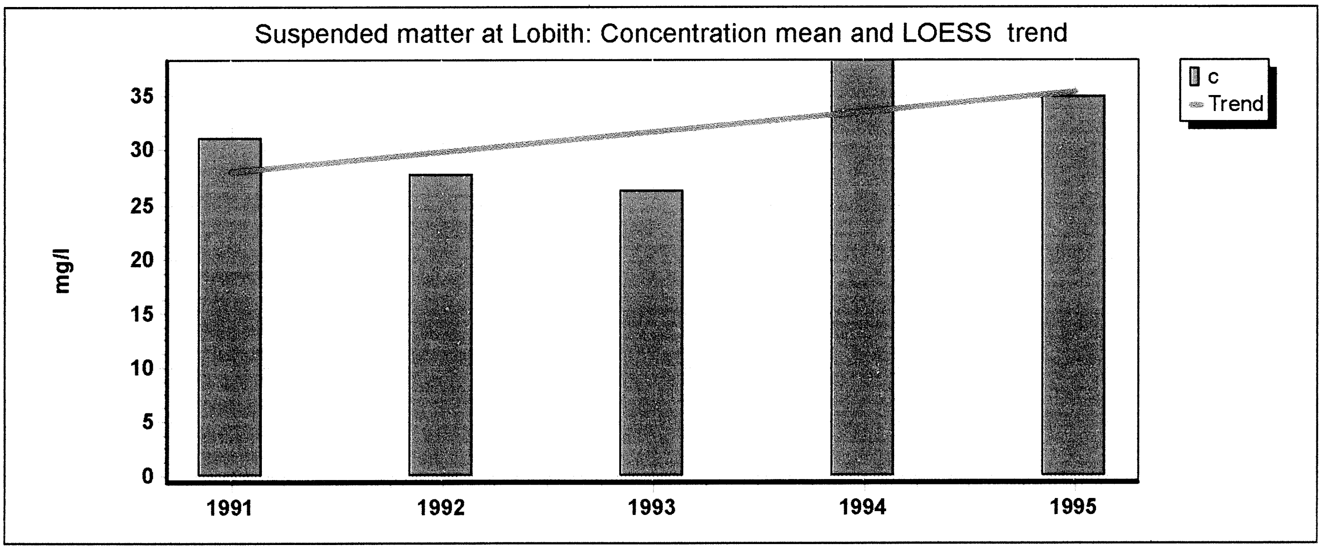

NO3-N at Lobith: Concentration mean and LOESS trend
mg/l
4,0
3,0
2,0
1,0
0,0
1955
1960
1965
1970
1975
1980
1985
1990
1995
c
Trend



Suspended matter at Lobith: Multiplicatively adjusted loads
1000 t/a
4.500
4.000
3.500
3.000
2.500
2.000
1.500
1.000
500
0
1991
1992
1993
1994
1995
A0
N
H
L1
L2
L3
L4
S1
S2
BC
OSPAR



Suspended matter at Lobith: Trend of adjusted loads
1000 t/a
4.000
3.500
3.000
2.500
2.000
1.500
1.000
500
0
1991
1992
1993
1994
1995
OSPAR
A0
N
H
L1
L2
L3
L4
S1
S2



Suspended matter at Lobith: Concentration mean and LOESS trend
mg/l
35
30
25
20
15
10
5
0
1991
1992
1993
1994
1995
c
Trend

Annex B

Complements and further explanations

Contents

B 1 Interpretation of the adjusted load

In this section the interpretion of the adjustment concept and the interpretation of adjusted loads will be discussed in detail.

The measured input loads are composed of many different contributions, which can be seen as caused by a set of more or less fixed sources, such as households, industry, farming, area geology etc. Adjustment of inputs according to natural variations has to take into account the different nature of these sources. If e.g. 80% of the load is not affected by natural variations since it is caused by point sources, only for the remaining 20% of the load an adjustment is sensible. For special cases the adjusted input can be calculated as follows.

Point sources only

Assume that there are only point sources, i.e. assume inputs are not affected by climatic variation. Then no adjustment is required, i.e. the adjusted load $L_{ij,a}$ should be equal to the actual load, i.e. $L_{ij,a} = L_{ij}$.

Constant concentration not depending on the runoff

Assume that there are only diffuse sources, causing constant concentrations not depending on the runoff. Then the load L_{ij} is proportional to the runoff and it can be adjusted by multiplying with q_{0ij} / q_{ij}, i.e. $L_{ij,a} = L_{ij}\, q_{0ij} / q_{ij}$.

Adjustment of a mixture of loads of two sources

Assume that 30%, say, of the load is caused by point sources and 70% by loads with constant concentration, then the aggregated adjusted load should be the sum of the single adjusted loads, i.e. $L_{ij,a} = 0.3\, L_{ij} + 0.7\, L_{ij}\, q_{0ij} / q_{ij} = (0.3 + 0.7\, q_{0ij} / q_{ij})\, L_{ij}$

If the percentages are known, no further calculation is needed. Otherwise the question arises how to calculate the percentage of the load due to diffuse sources and due to point sources. If the CQ function is known, the percentages can be calculated as follows: Under the conditions prescribed the CQ function can be written

$$c_{ij}(q) = \frac{\alpha_{ij}}{q} + \beta_{ij}$$

and therefore the LQ function (load runoff function) equals

$$c_{ij}(q)q = f_{ij}(q) = \alpha_{ij} + \beta_{ij}q$$

where α_{ij} denotes the load due to point sources and $\beta_{ij}q$ denotes the load due to diffuse sources. Hence the percentage of load due to diffuse sources can be calculated

$$\frac{\beta_{ij}q}{\alpha_{ij} + \beta_{ij}q}$$

and the percentage of load due to point sources can be calculated

$$\frac{\alpha_{ij}}{\alpha_{ij} + \beta_{ij}q} .$$

According to this approach the adjusted load can formally be written

$$L_{ij,a} = \frac{\alpha_{ij}}{\alpha_{ij} + \beta_{ij}q_{ij}} L_{ij} + \frac{\beta_{ij}q_{ij}}{\alpha_{ij} + \beta_{ij}q_{ij}} L_{ij} \frac{q_{0j}}{q_{ij}} = \frac{\alpha_{ij} + \beta_{ij}q_{0j}}{\alpha_{ij} + \beta_{ij}q_{ij}} L_{ij} = \frac{L_{ijm}}{L_{ije}} L_{ij} .$$

This formula means that the adjusted load simply can be calculated by multiplying the actual load with the ratio of estimated load at mean runoff and the estimated load at actual runoff, and in case of 70% load due to diffuse sources this multiplication factor equals (0.3+ 0.7 q_{0j} / q_{ij}).

Nonlinear LQ Function

Assume that the load follows the LQ function

$$L_{ij} = f_{ij}(q_{ij}) = \gamma_{ij}q_{ij}^{d}$$

with parameters γ_{ij} and d. Adjustment means that the actual runoff q_{ij} will be replaced by the long term mean runoff q_{0ij}. Since $\gamma_{ij} = \frac{L_{ij}}{q_{ij}^d}$, this leads to

$$L_{ij,a} = \gamma_{ij} q_{0j}^d = \frac{q_{0j}^d}{q_{ij}^d} L_{ij} = \frac{f\left(q_{0j}^d\right)}{f\left(q_{ij}^d\right)} L_{ij} .$$

This means again that the adjusted load simply can be calculated by multiplying the actual load with the ratio of estimated load at mean runoff and the estimated load at actual runoff.

Adjustment of a mixture of loads of three sources

Assume that 30%, say, of the load is caused by point sources, 50% by sources causing constant concentration and 20% by sources causing a non-linear load-runoff function, then the aggregated adjusted load should be the sum of the single adjusted loads, i.e.

$$L_{ij,a} = 0.3\ L_{ij} + 0.5\ L_{ij}\ q_{0j}\ /\ q_{ij} + 0.2\ L_{ij}\ (q_{0ij}\ /\ q_{ij}\ )^d$$

If the percentages are known, no further calculation is needed. Otherwise the question arises how to calculate them. As in section 2.3, if the CQ function is known, the percentages can be derived from the CQ or the LQ function, respectively: Under the conditions prescribed the LQ function can be written

$$c_{ij}(q)q = \alpha_{ij} + \beta_{ij} q + \gamma_{ij} q^d$$

where α_{ij} denotes the load due to point sources, $\beta_{ij} q$ denotes the load due to diffuse sources (linear), and $\gamma_{ij} q^d$ denotes the load due to the non-linear component. Then the percentages of load due to point sources can be calculated

$$\frac{\alpha_{ij}}{\alpha_{ij} + \beta_{ij} q + \gamma_{ij} q^d},$$

the percentage of load due to diffuse sources can be calculated

$$\frac{\beta_{ij} q}{\alpha_{ij} + \beta_{ij} q + \gamma_{ij} q^d}$$

the percentage of load due to the non-linear component can be calculated

$$\frac{\gamma_{ij} q^d}{\alpha_{ij} + \beta_{ij} q + \gamma_{ij} q^d}$$

According to this approach the adjusted load can formally be written

$$L_{ij,a} = \frac{\alpha_{ij}}{\alpha_{ij} + \beta_{ij} q_{ij} + \gamma_{ij} q_{ij}^d} L_{ij} + \frac{\beta_{ij} q_{ij}}{\alpha_{ij} + \beta_{ij} q_{ij} + \gamma_{ij} q_{ij}^d} L_{ij} \frac{q_{0ij}}{q_{ij}} + \frac{\gamma_{ij} q_{ij}^d}{\alpha_{ij} + \beta_{ij} q_{ij} + \gamma_{ij} q_{ij}^d} L_{ij} \left(\frac{q_{0ij}}{q_{ij}} \right)^d$$

$$= \frac{\alpha_{ij} + \beta_{ij} q_{0ij} + \gamma_{ij} q_{0ij}^d}{\alpha_{ij} + \beta_{ij} q_{ij} + \gamma_{ij} q_{ij}^d} L_{ij} = \frac{L_{ijm}}{L_{ije}} L_{ij}.$$

Again, this is in accordance with the definition of the adjusted load used in this report in section 2.2.

Interpretation of aggregated adjusted loads

In this subsection the interpretation of the annual adjusted load is investigated The annual adjusted load can be obtained by taking the mean of the individual loads. If there are n samples measured in year i, the annual adjusted load – assuming a linear LQ function - can be computed

$$L_{ia} = \frac{1}{n_i} \sum_{j=1}^{n_i} L_{ija} = \frac{1}{n_i} \sum_{j=1}^{n_i} \left(\frac{\alpha_{ij}}{\alpha_{ij} + \beta_{ij} q_{ij}} L_{ij} + \frac{\beta_{ij} q_{ij}}{\alpha_{ij} + \beta_{ij} q_{ij}} L_{ij} \frac{q_{0ij}}{q_{ij}} \right)$$

$$= \frac{1}{n_i} \sum_{j=1}^{n_i} \left(\frac{\alpha_{ij} c_{ij}}{\alpha_{ij} + \beta_{ij} q_{ij}} q_{ij} + \frac{\beta_{ij} q_{ij} c_{ij}}{\alpha_{ij} + \beta_{ij} q_{ij}} q_{0ij} \right).$$

The components of this expression may be interpreted as follows: $c_{ij}^{*} := \dfrac{\alpha_{ij} c_{ij}}{\alpha_{ij} + \beta_{ij} q_{ij}}$ represents the concentration due to point sources, whereas $c_{ij}^{+} := \dfrac{\beta_{ij} q_{ij} c_{ij}}{\alpha_{ij} + \beta_{ij} q_{ij}}$ represents the concentration due to diffuse sources. Separate aggregation results in

$$L_{ia} = \frac{1}{n_i} \sum_{j=1}^{n_i} \left(c_{ij}^{*} q_{ij} + c_{ij}^{+} q_{0ij} \right) = \frac{1}{n_i} \sum_{j=1}^{n_i} c_{ij}^{*} q_{ij} + \frac{1}{n_i} \sum_{j=1}^{n_i} c_{ij}^{+} q_{0ij} = L_{i,a}^{*} + L_{i,a}^{+},$$

where

$$L_{ia}^{*} = \frac{1}{n_i} \sum_j c_{ij}^{*} q_{ij} = \left(\sum_j \frac{q_{ij}}{q_i} c_{ij}^{*} \right) q_i \,, \qquad \text{(Load due to point sources)}$$

$$L_{ia}^{*} = \frac{1}{n_i} \sum_j c_{ij}^{+} q_{0ij} = \left(\sum_j \frac{q_{0ij}}{q_{0i}} c_{ij}^{+} \right) q_{0i} \,, \qquad \text{(Load due to diffuse sources)}$$

$$q_i := \frac{1}{n_i} \sum_j q_{ij} \qquad \text{(mean runoffi in year } i\text{)}$$

$$q_{0i} := \frac{1}{n_i} \sum_j q_{0ij} \,. \qquad \text{(long term mean runoff).}$$

Both components of the adjusted annual load can be represented as a product of runoff and runoff corrected concentrationen, and the difference between the adjusted annual load and the „measured“ annual load can be calculated

$$L_i - L_{ia} = \left(\sum_j \frac{q_{ij}}{q_i} c_{ij}^{+} \right) q_i - \left(\sum_j \frac{q_{0ij}}{q_{0i}} c_{ij}^{+} \right) q_{0i} \,.$$

i.e. the difference can be explained by the difference between the actual runoff and the long term mean of the runoff.

B 2 Estimation methods

In the following the description of the estimation methods introduced in chapter 5 will be extended by more details.

B 2.1 Non-Parametric Smoothing (Method N)

B 2.1.1 Stalnacke's Recommendation

As per a recommendation put forth by Stalnacke (1996; see also the OSPAR Guidelines for Harmonised Quantification and Reporting Procedures for Nutrients – HARP-NUT – Guideline Number 7 : Quantification of the Total Riverine Load of Nutrients, 2000), the load is linearly modelled as per the following equation:

$$L_{ij} = \alpha_j + \beta_{ij} q_{ij} + \varepsilon_{ij},$$

where L_{ij} = load in year i and season j

q_{ij} = runoff in year i and season j

$i = 1,\ldots,d$

$j = 1,\ldots,m$

The index i denotes the year of measurement, while j indicates the season. The Stalnacke model requires a firm time-frame, that is to say, the season index j refers to a particular month in the year. This makes it necessary to first of all appropriately arrange all the measurement values within the given frame during data processing.

The model parameters α_j and βij are estimated by minimising an expression of the form:

$$S(\alpha,\beta) = \sum_{i,j} (L_{ij} - \alpha_j - \beta_{ij} q_{ij})^2 + \lambda_1 \sum_{i,j} (\beta_{ij} - \frac{\beta_{i+1,j} + \beta_{i-1,j}}{2})^2 + \lambda_2 \sum_{i,j} (\beta_{ij} - \frac{\beta_{i,j+1} + \beta_{i,j-1}}{2})^2 .$$

Sums are taken over all possible index combinations i,j, with

$\beta_{i,0} = \beta_{i-1,M}$ and

$\beta_{i,M+1} = \beta_{i+1,1}$

The first part of the sum represent the sum of squared residuals, whereas the second and the third componentspenalize non-linear changes of the paramter β: The second component penalizes nonlinear changes between years, and the third component penalizes nonlinear changes within the year. λ_1, λ_2 represent the corresponding penalty parameters. Suitable levels of the penalty factors can be established by undertaking a cross-validation study of relationships between L_{ij} and q_{ij}.

However, possibilities of using this model appear limited since only the proportional parameter β and not the constant component α is dependent on index i, that is to say, this load component – which in first approximation is determined by the point sources – does indeed contain a seasonal component but is however assumed to be temporally constant over the years. This assumption appears to be not quite satisfactory, at least in cases where there is a considerable reduction in inputs from point sources, possibly giving rise to considerable distortions in the adjusted load. It is for this reason that an extended non-parametric model is being examined as part of the present investigation.

B 2.1.2 An Extended Non-Parametric Model

The following model is considered is as an extension of the recommendation made by Stalnacke :

$$L_{ij} = \alpha_{ij} + \beta_{ij} q_{ij} + \varepsilon_{ij}.$$

with L_{ij} = load in year i and season j

q_{ij} = runoff in year i and season j

$i=1,\dots,T$

$j=1,\dots,M.$

This model differs from Stalnacke's recommendation in that not only β, but even α_{ij} is dependent on the year i. The two model parameters α_{ij} and β_{ij} can be non-parametrically estimated by minimizing the following equation:

$$S(\alpha,\beta)=\sum_{i,j}(L_{ij}-\alpha_{ij}-\beta_{ij}q_{ij})^2+\lambda_1\sum_{i,j}(\alpha_{ij}-\frac{\alpha_{i+1,j}+\alpha_{i-1,j}}{2})^2+\lambda_2\sum_{i,j}(\alpha_{ij}-\frac{\alpha_{i,j+1}+\alpha_{i,j-1}}{2})^2,$$

$$+\lambda_1\overline{q^2}\sum_{i,j}(\beta_{ij}-\frac{\beta_{i+1,j}+\beta_{i-1,j}}{2})^2+\lambda_2\overline{q^2}\sum_{i,j}(\beta_{ij}-\frac{\beta_{i,j+1}+\beta_{i,j-1}}{2})^2$$

where $\overline{q^2}=\frac{1}{N}\sum_{ij}q_{ij}^2$ denotes the arithmetical mean of the squared runoff.

This model can be extended by further parameters (eg. by a quadratic term). The functional S(α,β) can be interpreted as a quadratic form of a vector which is linear in α and β. If the quadratic form is positive definite (if not too many observations are missing), there is a unique minimum, and the corresponding estimates for α and β are linear in the measured loads L_{ij}.

Suitable levels of the penalty parameters λ_1, λ_2 can be established by undertaking a cross-validation study of relationships between L_{ij} and q_{ij}, however, for small data sets this will not lead to satisfying results. With the fixing of $\lambda_1 = \lambda_2$, seasonal changes in the parameters receive the same weight as changes recorded from year to year.

In order to obtain the desired degree of adjustment of the function, the number of generalized degrees of freedom is prescribed as per Hastie and Tibshirani (1990), this number being construable as the equivalent of the number of underlying parameters and equals the trace of the smoother matrix. This is the matrix which corresponds to the linear function between the vector of observed loads L_{ij} and the vector of estimated loads $\hat{L}_{ij}=\hat{\alpha}_{ij}+\hat{\beta}_{ij}q_{ij}$ beschreibt. The trace of the smoother matrix depends in a complex nonlinear way on $\lambda_1 = \lambda_2$, and an iterative procedure is required to compute $\lambda_1 = \lambda_2$ for a given trace (degrees of freedom). With 5-15 degrees of freedom satisfying fits could be achieved. For very long time series with more than 20 years a local use of the method is recommeded.

According to this model the multiplicatively adjusted load can be calculated

$$L_{ij,a}=\frac{\alpha_{ij}+\beta_{ij}q_{0j}}{\alpha_{ij}+\beta_{ij}q_{ij}}L_{ij}=\frac{\frac{\alpha_{ij}}{\beta_{ij}}+q_{0j}}{\frac{\alpha_{ij}}{\beta_{ij}}+q_{ij}}L_{ij}\ ,$$

i.e. the adjustment step is only depending on the ratio α_{ij}/β_{ij}, but not on the parameters itselves.

B 2.2 Application of Hebbel's Method of Estimation (Method H)

On the basis of Hebbel's method (1992) for dividing up time series into trend, season and exogenous effects, the following model may be used for recording the concentration – runoff relation :

$$c_t = u_t + s_t + \beta / q_t + \varepsilon_t$$

where c_t = concentration at the point of time t

L_t = load / transport at the point of time t

q_t = runoff at the point of time t

u_t = trend component

s_t = season component

β = effect of runoff on concentration (constant in time)

As opposed to the model recommended by Stalnacke, the measurement times $t_1,...,t_n$ during the measuring period under consideration are not necessarily equidistant.

Alternatively one could model trend and season not for the concentration, but for the load, and to consider the model

$$L_t = u_t + s_t + \beta \times q_t + \varepsilon_t.$$

However, calculation performed by way of trial were not satisfying and therefore the load model was not considered any more.

Parameters for the model introduced at the beginning are determined on the basis of the minimization of a smoothness measurement which is defined through an appropriately fixed trend-season differential operator. It can be derived from the case without exogen variables. Assuming β to be known, one computes $z_t = L_t/q_t - \beta/q_t$ and calculates trend and season for the model

$$z_t = u_t + s_t + \varepsilon_t$$

Since the estimation procedure is linear, there is a smoother matrix W which describes the linear relation between the z_t und the estimation vector. This may be represented as $\hat{z} = Wz$, where z and $\hat{z}$ denote the vectors representing the components z_t and the estimated components, respectively.

Under the assumption that u+s is known, β can be estimated by linear regression of $v_t = L_t/q_t - (u_t + s_t)$ in the model

$$v_t = \beta \times q_t + \varepsilon_t \, .$$

and by combination of the partial solutions one obtains

$$\hat{z} = W\left(c - x'\hat{\beta}\right)$$

with $\hat{\beta} = \left(x'(I-W)x)\right)^{-1} x'(I-W)c\right)$,

where c denotes the vector of the concentrations $c_t = L_t/q_t$ and x the vector of the corresponding reciprocal runoff $1/q_t$.

For the calculations presented here this method was used together with a linear trend and a second order season component. The method is dependent on a smoothing parameter SIGMA which does not explicitly find its way into the CQ relation but to the abovementioned trend-season differential operator. In the absence of other predetermined parameters it was decided to fix this smoothing parameter SIGMA in such a way that the number of generalized degrees of freedom stands at 12. This means that in addition to the six parameters required for the underlying regression model, there are six parameters for the non-parametric part of the model. By way of trial a higher number of degrees was tested as well, but no significant improvements were observed with regard to the adjusted loads.

It may be noted that parameter β, which describes that portion of the load that is independent of runoff, remains constant in the model. But in order to nevertheless ensure a flexible adjustment to changed CQ relations the model is locally used, that is to say, the estimation takes place separately for every single point of time on the basis of all data within a running time window. A time window of 7 years proved to be favourable in the case of the evaluations, with the first or last seven years being considered at the beginning or end of a time series in each case, whereas in the middle region of the time series, the time window is so fixed that the point of time under investigation lies exactly in the middle of the time window. In case of non-availability of values the time window is accordingly stretched so that – in the case of monthly data – the time window encompasses exactly 7x12+1=85 individual values.

According to this model the multiplicatively adjusted load can be written

$$L_{t,a} = \frac{\beta + (u_t + s_t)q_{0t}}{\beta + (u_t + s_t)q_t} L_t = \frac{\frac{\beta}{u_t + s_t} + q_{0t}}{\frac{\beta}{u_t + s_t} + q_t} L_t ,$$

where q_{0t} denotes the long term mean in the month corresponding to t. This means that the adjustment is determined by the ratio $\beta/(u_t + s_t)$.

B 2.3 Local Regression with Season (Method L1)

If the prescribed value of six degrees of freedom were to be selected for Hebbel's method described in the foregoing section, then the estimation of the adjustment parameters will be equivalent to a regression estimate on the basis of the following linear model:

$$c_t = \frac{\alpha}{q_t} + \beta + \delta t + season + \varepsilon_t ,$$

with $season := \gamma_1 \sin\frac{2\pi t}{m} + \gamma_2 \cos\frac{2\pi t}{m} + \gamma_3 \sin\frac{2\pi t}{2m} + \gamma_4 \cos\frac{2\pi t}{2m}$

denoting the season component. Further m represents the length of the year, expressed in the unit of measurement used for the time t. It should be pointed out that as per this model, concentration follows a linear trend, while the effect of runoff on concentration remains constant in time. Both this model as well as Hebbel's method are appropriately used on the basis of a running time window of 7 years in keeping with the objective at hand. In case of non-availability of values, the time-window will be accordingly extended so that it encompasses exactly 7x12+1=85 individual values in terms of monthly data.

With this model the multiplicatively adjusted load can be written

$$L_{t,a} = \frac{\alpha + (\beta + \delta t + season)q_{0t}}{\alpha + (\beta + \delta t + season)q_t} L_t$$

$$= \frac{\alpha/(\beta + \delta t + season) + q_{0t}}{\alpha/(\beta + \delta t + season) + q_t} L_t$$

where q_{0t} denotes the long term mean of the runoff in the month corresponding to t.

B 2.4 Local Regression with Season and Lagged Runoff Effect (Method L2)

The CQ relation is more often than not dependent on not just the current runoff but also on earlier runoff. Experience has shown here that higher concentrations should be expected with increasing runoff and lower concentrations with decreasing runoff. It therefore follows that the model described in the foregoing section be extended for a lagged runoff effect as below:

$$c_t = \frac{\alpha}{q_t} + \frac{\gamma}{q_{t-1}} + \beta + \delta t + season + \varepsilon_t$$

where q_{t-1} represents the runoff measured on the previous day, and *season* is defined as in the previous section. It should be noted here that often a runoff value is available on day t-1 though there is generally no concentration value, for concentration measurements are typically enough carried out in approximation on a biweekly or monthly basis.

Due to the higher number of parameters and the consequently somewhat lower stability of the estimation values, it proved useful to extend the window during regression estimation from 7 to 8 years. This means that a higher flexibility in model adjustment is obtained at the cost of a somewhat lower temporal flexibility.

With this model the multiplicatively adjusted load can be written

$$L_{t,a} = \frac{\alpha + \gamma + (\beta + \delta t + season)q_{0t}}{\alpha + \gamma \frac{q_t}{q_{t-1}} + (\beta + \delta t + season)q_t} L_t$$

$$= \frac{(\alpha + \gamma)/(\beta + \delta t + season) + q_{0t}}{\left(\alpha + \gamma \frac{q_t}{q_{t-1}}\right)/(\beta + \delta t + season) + q_t} L_t$$

where q_{0t} denotes the long term mean of the runoff in the month corresponding to t.

Therefore the adjusted load depends on both trend and season, $\beta + \delta t + season$, and the parameters α und γ. γ should be positive: Then swelling of the runoff implies a reduction of the adjusted load.

B 2.5 Local Regression with Temperature and Lagged Runoff Effect (Method L3)

In order to obtain a – as far as possible – simple modelling of the CQ relation, the option that seems logical is to substitute the season modelling through a temperature effect which possibly reflects a similar trend for the year. Thus the following CQ relation is obtained in amendment of the model described in Section 5.5:

$$c_t = \frac{\alpha}{q_t} + \frac{\gamma}{q_{t-1}} + \beta + \delta t + \eta w_t + \varepsilon_t$$

where w_t denotes the water temperature on day t. Both for this model as well as for Method L1, parameter estimation is based on a running time window, with the more instable behaviour of the estimation function (determined in preliminary tests) prompting the choice of a time-window extended to eight years.

With this model the multiplicatively adjusted load can be written

$$L_{t,a} = \frac{\alpha + \gamma + (\beta + \delta t + \eta w_t) q_{0t}}{\alpha + \gamma \frac{q_t}{q_{t-1}} + (\beta + \delta t + \eta w_t) q_t} L_t \ ,$$

i.e. the adjusted load depends on the parameters α, γ und the expression $\beta + \delta t + \eta w_t$.

B 2.6 Local Regression with Season, Temperature und Lagged Runoff Effect (Method L4)

If the two models described in Sections 5.5 and 5.6 are combined, then the following CQ relation is obtained:

$$c_t = \frac{\alpha}{q_t} + \frac{\gamma}{q_{t-1}} + \beta + \delta t + \eta w_t$$
$$+ \gamma_{1ij} \sin\frac{2\pi t_{ij}}{m} + \gamma_{2ij} \cos\frac{2\pi t_{ij}}{m} + \gamma_{3ij} \sin\frac{2\pi t_{ij}}{2m} + \gamma_{4ij} \cos\frac{2\pi t_{ij}}{2m} + \varepsilon_{ij}$$

where w_t again denotes the water temperature on day t. The parameter estimation of this model takes place on the basis of a running time window again with a duration of eight years.

The multiplicatively adjusted load can be computed

$$L_{t,a} = \frac{\alpha + \gamma + (\beta + \delta t + \eta w_t + season)q_{0t}}{\alpha + \gamma \frac{q_t}{q_{t-1}} + (\beta + \delta t + \eta w_t + season)q_t} L_t$$

where the season is defined as above.

B 2.7 Estimation Using Splines (Method S1)

The methods described above assume that the runoff-load relation is approximately linear. In the case of parameters for which this approximation is not justified, a flexible adjustment of the CQ relation could be obtained using a cubic spline. The calculation of this cubic spline may be understood as linear smoothing, with the smoothing parameter being fixed through the degrees of freedom, that is to say, the course of the linear representation (as per Hastie and Tibshirani's approach). A value of approximately 4 is prescribed for this course. If s denotes the spline function, then the CQ relation can be expressed as:

$$c_t = s(q_t) + \varepsilon_t$$

Method S1 is based on the assumption that the spline is determined on the basis of all available measurement values, in other words what is assumed is a global, trend-free dependence between runoff and concentration. An assumption of this nature in certainly not appropriate for long series, but for short series which are not longer than 7 or 8 years, the assumption of a statistical CQ relation for load adjustment appears to be a simple and practicable method. The multiplicatively adjusted load at time t may be expressed as follows:

$$L_{t,a} = \frac{s(q_{0t})q_{0t}}{s(q_t)q_t} L_t \ ,$$

In other words, apart from the relation between the current runoff q_t and the long-term runoff mean q_{0t} the relation between the spline values at the points q_t and q_{0t} is crucial for adjustment.

B 2.8 Estimation Using Local Splines (Method S2)

In order to represent temporal trends more efficiently it is recommended that the spline calculation not be carried out globally but that a window technique be used here too as with methods L1 to L4. A small data window would suffice since no further parameters are to be considered. Thus for method S2 a window with a span of three years was used for spline calculation.

B 3 Calculation of adjusted loads based on the annual sample

B 3.1 Use of the prediction value of the LQ function

An alternative adjustment approach consists in estimating the LQ function using the data collected in that particular year and then to use the predicted value of the LQ function for the long term mean run-off. This procedure was discussed by WGSAEM and tested by using the time series of NO_3-N- and P_{Total} for Lobith/Rhine and Herbrum/Ems.

Let $(L_{ij}, q_{ij}), j=1,\ldots,m$, be the pairs of load and flow measurements in year i, and let q_0 be the mean flow over the entire time series.

Two LQ functions were fitted assuming gamma errors and identity link:

Y1: $L_{ij} = \alpha_i + \beta_i q_{ij} + \varepsilon_{ij}$, $j=1,\ldots,m$, with the predicted load $\hat{\alpha}_i + \hat{\beta}_i q_0$.

Y2: $L_{ij} = s_i(q_{ij}) + \varepsilon_{ij}$, $j=1,\ldots,m$, where $s_i(.)$ denotes a year-specific smoothing spline on 2 degrees of freedom that allows for a non-linear load-flow relationship with the predicted load $s(q_0)$.

B 3.2 Comparison of results

To assess the performance of the methods, the residual standard deviation of the annual indices was calculated by fitting a LOESS smoother with a span of eight years (and corrected for differences in the mean level). For comparison, the residual standard deviation was also calculated for the method L1, which uses information from adjacent years. The results (in tonnes per year) given in Table B 3.1:

Table B 3.1: Residual standard deviations of the annual loads

	Rhine/Lobith		Ems/Herbrum	
	NO_3-N	P_{Total}	NO_3-N	P_{Total}
OSPAR	37412	3544	3586	226
Y1	12808	3241	2879	152
Y2	13002	2757	2083	152
L1	9076	2545	1300	115

In order to make the results comparable, a level correction of the results of method L1 is included. In terms of smoothness, method L1 performs best throughout. Method Y2 also performs reasonably across all four time series.

B 3.3 Interpretation as additively adjusted load

The results of method Y1 and Y2 are very similar. This refers to the interpretation of the methods as additively adjusted loads: The additively adjusted annual load based on the model

$$L_{ij} = \alpha_i + \beta_i \, q_{ij} + \varepsilon_{ij} \quad ,j=1,\ldots,m$$

can be calculated

$$\frac{1}{m}\sum_{j=1}^{m} L_{ija} = \frac{1}{m}\sum_{j=1}^{m}\left(L_{ij} - L_{ije} + L_{ijm}\right) = \frac{1}{m}\sum_{j=1}^{m}\left(L_{ij} - \left(\hat{\alpha}_i + \hat{\beta}_i q_{ij}\right) + \left(\hat{\alpha}_i + \hat{\beta}_i q_0\right)\right) = \hat{\alpha}_i + \hat{\beta}_i q_0,$$

since

$$\frac{1}{m}\sum_{j=1}^{m} L_{ij} = \frac{1}{m}\sum_{j=1}^{m}\left(\hat{\alpha}_i + \hat{\beta}_i q_{ij}\right).$$

The additively adjusted annual load based on the model

$$L_{ij} = s_i(q_{ij}) + \varepsilon_{ij} \quad ,j=1,\ldots,m,$$

can be computed

$$\frac{1}{m}\sum_{j=1}^{m} L_{ija} = \frac{1}{m}\sum_{j=1}^{m}\left(L_{ij} - L_{ijc} + L_{ijm}\right) = \frac{1}{m}\sum_{j=1}^{m}\left(L_{ij} - s_i\left(q_{ij}\right) + s_i\left(q_0\right)\right) = s_i\left(q_0\right).$$

This means that the loads calculated with the methods Y1 and Y2 are additively adjusted loads based on a linear LQ function and a spline function, respectively.

B 3.4 Is the adjusted load calculated with Y1 or Y2 autocorrelated?

The annual loads calculated with the methods Y1 and Y2 are determined by the data collected in that particular year. Therefore the annual loads are stochastically independent if the underlying runoff and concentration series are uncorrelated. Otherwise the autocorrelation in the runoff can induce considerable autocorrelation in the adjusted annual load. This is demonstrated in the following hypothetical example.

It is assumed that there is no measurement error and that there are two measurements only in each year. The LQ function in winter is given by

$$L = \alpha_w + \beta_w q$$

and in summer by

$$L = \alpha_s + \beta_s q.$$

It is assumed that both LQ functions keep constant over the years. Furthermore, q_{is} denotes the runoff in summer and q_{iw} the runoff in winter in year i. Then the coefficients of the LQ function

$$L_{ij} = \alpha_i + \beta_i q_{ij} + \varepsilon_{ij}$$

can be represented by

$$\alpha_i + \beta_i q_{iw} = \alpha_w + \beta_w q_{iw}$$
$$\alpha_i + \beta_i q_{is} = \alpha_s + \beta_s q_{is}$$

The LQ function can be represented graphically by connecting the points (q_{iw} , $\alpha_w + \beta_w q_{iw}$) and ($q_{is}$, $\alpha_s + \beta_s q_{is}$) by a straight line. In Fig. B 9.1 it is assumed that the LQ function in winter is given by

$$L = 0{,}8 + 0{,}2\, q$$

and in summer by

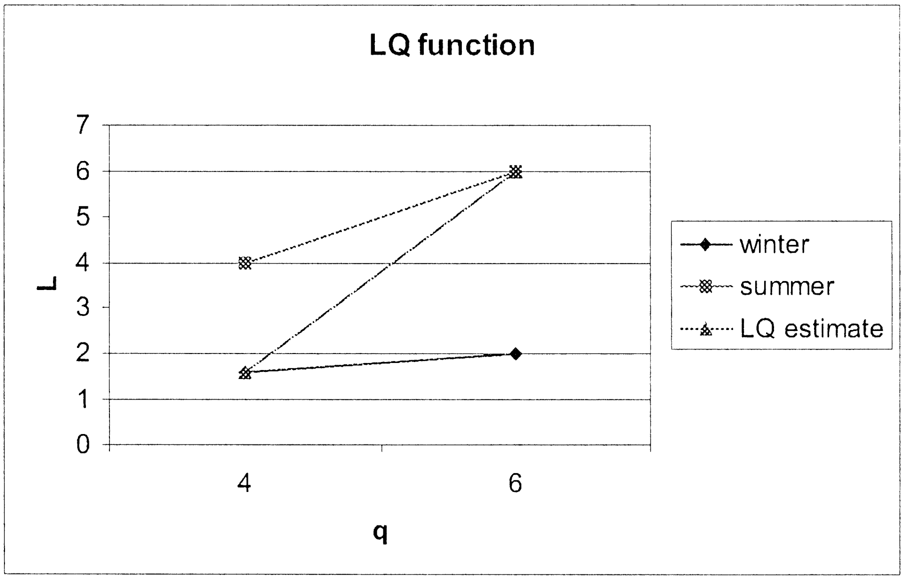
$$L = q.$$

It is assumed that the runoff in the current year is given by $q_{iw} = 4$ and $q_{is} = 6$. Then the LQ function can be calculated

$$L = -7{,}2 + 2{,}2\, q.$$

If the long term mean runoff equals $q_0 = 3$, the adjusted load will be negative, $\alpha_i + \beta_i q_0 = -0{,}6$.

Figure B 3.1: Seasonal variation in the LQ function may induce autocorrelation in the loads calculated with the methods Y1 and Y2, respectively.



If the runoff in summer is changed to $q_{is} = 3$, the slope of the LQ function will be negative and the adjusted load will be =3.

This demonstrates that seasonal variation of the LQ function and random fluctuation of the runoff may induce considerable variation of the adjusted load calculated with the method Y1 or Y2, respectively. This implies further that autocorrelation in the annual runoff may induce considerable autocorelation in the series of the annual adjusted loads calculated with Y1 or Y2.

The use of the methods Y1 and Y2 therefore can be recommended only if there is no seasonal variation in the LQ function. Otherwise a correction for the seasonal effect is necessary in order to avoid the effects described above.

B 4 Autocovariance of the adjusted annual load

For the statistical evaluation of the adjustment relevant especially important is the covariance matrix of the load series. An adjustment should guarantee that the variance is small and that covariances are neglectable. The latter is a prerequisite for a trend analysis based on the annual adjusted loads.

The following calculations are based on additively adjusted loads, which can be considered as first order approximations of multiplicatively adjusted loads. Additively adjusted loads allow detailed investigations of statistical properties. The estimators described in chapter 2 are linear in the measured concentrations, and therefore the additively adjusted annual load is a linear function of the measured concentrations, too: The Vector $L_a = (L_{1a}, L_{2a}, \dots, L_{Ia})'$ of the additively adjusted annual loads $L_{ia} = L_i - L_{ie} + L_{im}$ can be written

$$L_a = S(Q)C$$

with a (IxN) matrix $S(Q)$, which depends on the runoff q_t , but not on the conzentrations c_t, whereas $C = (c_{t_1}, c_{t_2}, \dots, c_{t_N})'$ denotes the (Nx1) vector of the measured concentrations.

$C = (c_{t_1}, c_{t_2}, \dots, c_{t_N})'$ depends on the runoff, and therefore the following model is considered:

$$C = B(Q) + \varepsilon,$$

with $Cov(\varepsilon) = \sigma^2 I_N$ and unity matrix I_N. Assuming that the random vector ε and the random vector of the runoff $Q = (q_t)$ are stochastically independent, one obtains

$$Cov(L_a) = E[L_a L_a'] - E[L_a] E[L_a'], \quad \text{with}$$

$$E[L_a] = E[S(Q)C] = E[S(Q) B(Q)] \quad \text{and}$$

$$\begin{aligned} E[L_a L_a'] &= E[S(Q)CC' S(Q)'] = E[S(Q) B(Q) B(Q)' S(Q)'] + E[S(Q)\varepsilon\varepsilon' S(Q)'] \\ &= E[S(Q) B(Q) B(Q)' S(Q)'] + \sigma^2 E[S(Q) S(Q)']. \end{aligned}$$

It follows

$$Cov(L_a) = \sigma^2 E[S(Q) S(Q)'] + Cov(S(Q) B(Q)).$$

It should be noted that a prerequisite of this equation is the stochastical independence and homoscedasticity of the error term ε, and the stochastical independence of the runoff. In case of severe deviations of these assumptions a modification would be necesssary.

S(Q)B(Q) represents for the regression methods L1-L4 exactly and for the other methods approximately the vector of the estimated mean loads L_{im}, i.e.

$$S(Q)\, B(Q) = L_{im}\,.$$

These estimated mean loads are determined by the long term monthly mean of the runoff. Therefore the random fluctuations of the runoff do not affect $S(Q)B(Q)$ in a direct way, but only by estimation errors of the CQ function.

Therefore Cov(S(Q) B(Q)) is neglectable compared with the covariance matrix σ^2 E[S(Q) S(Q)'] which is determined by ε. Hence the covariance matrix of the vector of adjusted loads can be approximated

$$Cov(L_a) = \sigma^2 E[S(Q)\, S(Q)']$$

It should be noted that in this expression (Q) represents the stochastic process of the runoff. Therefore S(Q) represents a random matrix. For every realisation (q) of the stochastic process one may calculate the matrix S(q) and obtains the conditional covariance matrix

$$Cov(L_a|(q)) = \sigma^2 S(q)\, S(q)'$$

for the series of the runoff (q). This covariance matrix was computed for several estimation methods and several time series. Only small differences were observed between several estimation procedures, whereas the differences between different time series were significant. However in all cases the autocorrelation was small. Averaging the conditional covariance matrix Cov(L_a|(q)) over many realisations (q) results asymptotically in the covariance matrix Cov(L_a).

B 4.1 Covariances of the adjusted annual load at Lobith and Herbrum

The flow data series from Lobith/Rhine 1973-1995 was used to calculate the covariance matrix of the annual (additive-) adjusted loads according to method L1, and assuming a time window of 10 years with 26 measurements each year. The covariance matrix is shown below, in units of $(100\sigma \times m^3/s)^2$.

27.7	1.0	0.8	0.4	0.2	-0.0	-0.2	-0.1	-0.2	-0.1
1.0	28.2	0.2	0.2	0.0	-0.1	-0.2	-0.1	-0.0	-0.1
0.8	0.2	28.8	-0.4	-0.1	0.1	-0.1	-0.1	-0.0	-0.0
0.4	0.2	-0.4	29.5	-0.5	-0.1	0.3	0.1	-0.2	-0.3
0.2	0.0	-0.1	-0.5	29.6	-0.5	0.0	0.2	-0.0	-0.0
-0.0	-0.1	0.1	-0.1	-0.5	29.1	-0.3	0.1	0.4	0.2
-0.2	-0.2	-0.1	0.3	0.0	-0.3	28.2	0.0	0.5	0.7
-0.1	-0.1	-0.1	0.1	0.2	0.1	0.0	27.7	0.5	1.2
-0.2	-0.0	-0.0	-0.2	-0.0	0.4	0.5	0.5	28.8	1.0
-0.1	-0.1	-0.0	-0.3	-0.0	0.2	0.7	1.2	1.0	28.8

There is slightly negative correlation in the middle of the time series, and slightly positive correlation at start and beginning, but the correlation is below 3.5%. With the long term annual mean runoff 2320 m^3/s, the relative standard deviation of the adjusted load equals

$$\sigma_{rel} \frac{\sqrt{28 \times 10000}}{2320} = 0,228\, \sigma_{rel},$$

where σ_{rel} the relative standard deviation of the measured concentrations. σ_{rel} can be estimated by the corresponding relative residual standard deviation.

Under the assumption of monthly measurements the covariance matrix of the annual adjusted loads is as follows, in the unit $(100\sigma \times m^3/s)^2$.

59.5	2.3	1.9	0.8	0.3	-0.1	-0.5	-0.2	-0.4	-0.4
2.3	60.7	0.5	0.5	0.1	-0.2	-0.4	-0.3	-0.2	-0.3
1.9	0.5	61.9	-0.8	-0.0	0.3	-0.2	-0.3	-0.2	-0.1
0.8	0.5	-0.8	63.4	-1.1	0.0	0.7	0.3	-0.4	-0.5
0.3	0.1	-0.0	-1.1	63.7	-1.0	0.1	0.4	0.0	0.0
-0.1	-0.2	0.3	0.0	-1.0	62.8	-0.6	0.4	0.9	0.5
-0.5	-0.4	-0.2	0.7	0.1	-0.6	60.9	0.1	1.2	1.8
-0.2	-0.3	-0.3	0.3	0.4	0.4	0.1	60.0	1.3	2.7
-0.4	-0.2	-0.2	-0.4	0.0	0.9	1.2	1.3	62.1	2.4
-0.4	-0.3	-0.1	-0.5	0.0	0.5	1.8	2.7	2.4	62.2

The correlation structure is very similar to the correlation structure based on 26 measurements in the year. The maximum correlation is below 4% and therefore neglectable. However, the variance is considerably higher, $10000 \times \sigma^2 \times 61$ $[(m^3/s)^2]$, and the relative standard deviation of the adjusted annual load equals

$$\sigma_{rel} \frac{\sqrt{61 \times 10000}}{2320} = 0{,}337\, \sigma_{rel}\,.$$

The flow data series from Herbrum/Ems 1980-1997 yields the following covariance matrix, in the unit $100 \text{x} \sigma^2$:

13.06	-0.26	0.04	0.01	-0.06	-0.02	0.03	0.02	-0.06	-0.05
-0.26	12.56	0.02	0.10	0.10	-0.03	-0.05	-0.00	0.02	-0.04
0.04	0.02	11.74	0.06	0.17	0.18	0.08	-0.08	0.00	0.03
0.01	0.10	0.06	11.64	0.10	0.21	0.22	-0.06	-0.13	-0.07
-0.06	0.10	0.17	0.10	11.38	0.11	0.14	0.11	-0.02	0.00
-0.02	-0.03	0.18	0.21	0.11	11.75	-0.08	-0.01	0.27	0.09
0.03	-0.05	0.08	0.22	0.14	-0.08	13.77	-0.42	0.21	0.30
0.02	-0.00	-0.08	-0.06	0.11	-0.01	-0.42	14.40	-0.07	0.42
-0.06	0.02	0.00	-0.13	-0.02	0.27	0.21	-0.07	13.09	0.39
-0.05	-0.04	0.03	-0.07	0.00	0.09	0.30	0.42	0.39	12.63

The correlation is even smaller than for the Rhine. This can be explained by the higher range of variation for the River Ems, which allow a better estimation of the CQ function.

With the long term annual mean runoff 93 m^3/s, the relative standard deviation of the adjusted load equals

$$\sigma_{rel} \frac{\sqrt{13 \times 100}}{93} = 0{,}388\, \sigma_{rel}\,,$$

i.e. the relative standard deviation of the adjusted load for the River Ems is higher than for the River Rhine. This is due to large seasonal variation at the River Ems: The load is dominated by the input during the winter months, and therefore sampling errors in winter may affect the annual load considerably.

B 4.2 Trend analysis based on adjusted annual loads

A prerequisite of a trend analysis of the annual adjusted loads is that autocorrelation induced by the adjustment step is neglectable.

In the preceding section the covariance matrix was calculated for adjusted annual loads over a time span of 10 years. It appeared that the autocorrelation is below 4%. The consequences of this autocorrelation were examined by several simulation studies. It turned out the type I error for method L1 increases from 5% to 5,5% and 5,6% for Lobith/Rhine (with 26 and 12 measurements per year, respectively), and to 5,4% for Herbrum/Ems (with 12 measurements per year). In practise this cannot be detected and can therefore be neglected.

These calculations assume that the underlying statistical model holds. However, even if there are slight model deviations, eg. in case of slight non-linearity of the LQ function, the resulting autocorrelation will be neglectable.

If the components of ther error term ε are autocorrelated, both adjusted and unadjusted loads are autocorrelated too. This may be demonstrated by an example. Assuming monthly measurements at Lobith and a time series of 10 years, the average variance of the non-adjusted load equals 631.000 x σ^2 if there is no autocorrelation. The average variance of the correction term $L_{i,a}$ - L_i = - $L_{i,est}$ + $L_{i,mean}$ equals 28.000 x σ^2 (under the same assumptionsd, under model L1). This implies that the variation of the adjusted load is dominated by the variation of the unadjusted load.

If ε follows an autoregressive process AR(1) with rho=0.8, the variance for the unadjusted annual load increases to 3.150.000 x σ^2 , wheras the variance of the correction term increases less dramatically to 71410 x σ^2. In this case the variation of the adjusted load is almost completely determined by the variation of the unadjusted load.

Similar results were obtained for other stochastic processes. It can be concluded that the autocorrelation induced by the error term ε has the same order of magnitude for both adjusted and unadjusted annual loads. Since in practise of trend analysis the autocorrelation of unadjusted annual loads is neglected, the autocorrelation of adjusted annual loads may be neglected as well.

B 4.3 Autocorrelation of the OSPAR load

As demonstrated above, the covariance induced by the error term ε has the same order of magnitude for both adjusted and unadjusted loads. Unadjusted loads are additionally affected by the autocorrelation of the runoff. Even if there is no autocorrelation in ε, the runoff may induce considerable autocorrelation in the unadjusted annual loads (depending on the LQ function).

For the River Rhine it was calculated that the use of the OSPAR load for the analysis of trends increases the probability of a type one error from 5% to up to 17%. The latter holds especially in cases if the concentration is only slightly affected by the runoff (eg. for nitrate in the River Rhine) and if the random variation caused by ε is small compared with the variation of the annual runoff.

B 5 Lagged runoff effects

Adjustment of inputs aims in reducing the interannual variability of loads. However, adjustment is performed at the level of single measurements, whereas the interannual variability is based on aggregated values. As long as the CQ function is not depending on lagged runoff, this should not cause any problem. But what happens if there are lag effects?

In order to get a better understanding of possible lag effects, a simulation study applying a very simple simulation model was performed. It is assumed that daily measurements are available, and that the daily runoff is normally distributed according to the (unrealistic) model

$$q_{ij} = 6 + u_i + v_{ij}\,.$$

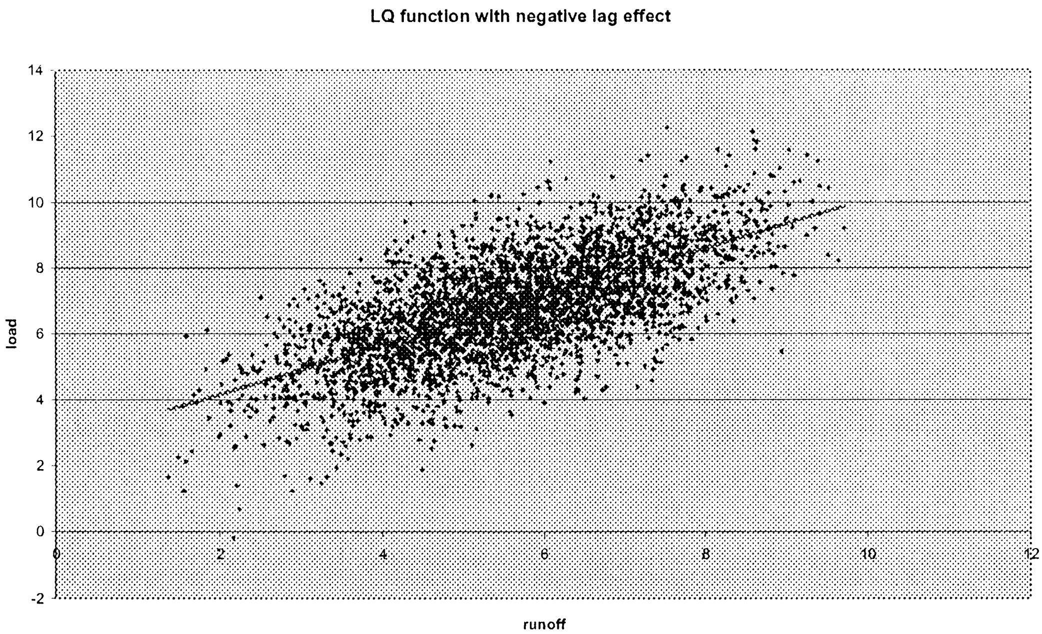
where u_i and v_{ij} denote random variables reflecting variations between years and within years. The measured load follows the model

$$L_{ij}=4+q_{ij}+p*q_{i,j-1}+ w_{ij}$$

where p denotes the lag effect of the runoff of the day before. All random variables u_i , v_{ij} und w_{ij} are stochastically independent and standard normally distributed. It should be noted that the mean load is constant over the years.

The simulation study was performed for 10 years and several p's. In each case the model parameters where calculated by using a simple regression approach, and then the adjusted loads were determinated. In case that there is no lag effect (p=0), this approach leads to substantial reduction of the interannual variability. But for very large lag effects this method may fail. Figure B 5.1 shows the resulting 3650 pairs of load and runoff obtained in the simulation study for p=-0.5:

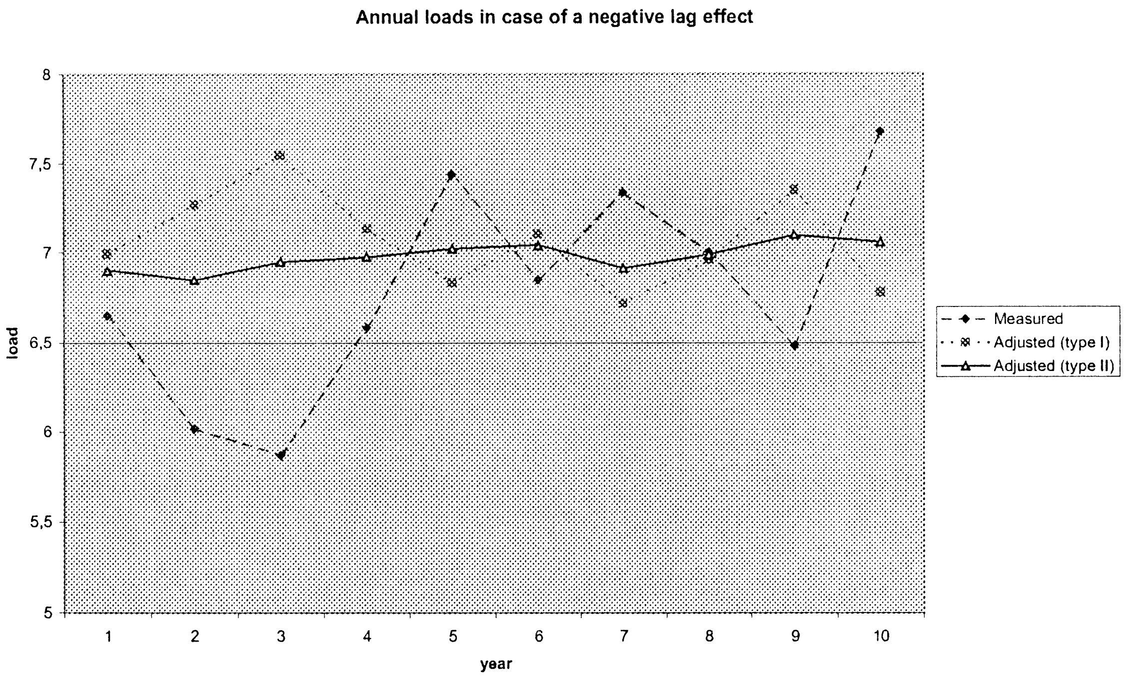
Figure B 5.1



The straight line represents the linear LQ function obtained from simple linear regression, not taking into account the negative lag effect. The resulting annual adjusted load is presented in Fig.B 5.2 (type I). It is clearly 'overadjusted'. This can be explained by the fact that the percentage of diffuse sources is overestimated when the negative lag effect is ignored. A better result can be explained when in the regression model the lag effect will be taken into account. The resulting adjusted load (type II) is almost constant over the years.

It can be concluded that lag effects of the runoff may lead to over-adjustment (in case of negative lag effects) as well as to under-adjustment (in case of positive lag effects), and in both cases the gain of adjustment may be deteriorated substantially. Therefore it is strongly recommended to check possible lag effects by calculating the correlation function between the residuals c_{ij}-c_{ij} (q_{ij}) and the lagged runoff $q_{i,j-r}$ for r=1,2,3,... If there is a significant correlation, the statistical model should be extended in a suitable manner.

Figure B5.2


Annual loads in case of a negative lag effect
8
7,5
7
6,5
6
5,5
5
load
1
2
3
4
5
6
7
8
9
10
year
Measured
Adjusted (type I)
Adjusted (type II)

B 6 Calculation of the power function

The power is calculated under the assumption that the linear trend is tested on the basis of the 7 year loess smoother. The test statistic can be written

$$T = b \ / \ (c \ s_{RES})$$

where

b = estimated slope (linear regression)
c = const, and

$$s_{RES} = \sqrt{\frac{1}{n-df} RSS} \ = \text{Residual standard deviation} \ .$$

RSS denotes the Sum of Squares of the Residuals based on the LOESS smoother, and df the trace of the smoother matrix. n denotes the number of years and c can be calculated

$$c = \frac{1}{\sum_{i=1}^{n}\left(i - \frac{n+1}{2}\right)^2} ,$$

It represents the variance of the estimator for the slope under the assumption the variance of the yearly (adjusted) loads equals 1. The slope b and the residual standard deviation s_{RES} depend on the measurement unit, and therefore

- the relative slope $b_{rel} = b \ / \ level$ and
- the relative residual standard deviation $s_{RES} \ / \ level$

are used for the calculation of the test statistic. *Level* represents the average load in the period of the time series.

If the data are stochastically independent and normally distributed, the test statistic T is non-central t-distributed with (n-df) degrees of freedom and non-centrality parameter

$$\delta = \frac{\beta}{\sigma}\sqrt{\sum_{i=1}^{n}\left(i - \frac{n+1}{2}\right)^2} \ .$$

If there is no trend, the non-central parameter vanishes and T is simply t-distributed with (n-df) degrees of freedom. Hence for testing the hypotheses

H_0: slope = 0
H_1: slope < 0

the null hypothesis can be rejected at significance level α if $T < -t_{n-df,1-\alpha}$. In case the slope is negative, the power function, i.e. the probability of rejection of the null hypothesis, can be calculated

$$p = F_{T_{n-df,\delta}}\left(-t_{n-df,1-\alpha}\right),$$

where $F_{T_{n-df,\delta}}$ denotes the cumulative distribution function of the non-central t-distribution with non-centrality parameter δ.

For the calculation of the power function the following assumptions are made: the number of years is n=10 and the significance level is α=0.05. If within these time span the reduction of inputs is 20%, the non-centrality parameter equals

$$\delta = \frac{-0{,}02}{s_{\mathrm{Res}} / Level}\sqrt{82{,}5} = \frac{-0{,}02}{s_{\mathrm{Res}} / Level} 9.083$$

and for a reduction of 50% the non-centrality parameter equals

$$\delta = \frac{-0{,}05}{s_{\mathrm{Res}} / Level}\sqrt{82{,}5} = \frac{-0{,}05}{s_{\mathrm{Res}} / Level} 9.083 .$$

For the relative residual standard deviation the data of past years may be used. In case of considerable changes of the level it is recommended to use the standard deviation of relative residuals instead of the relative residual standard deviation. This avoids overestimation of the true standard deviation.

The approach used here is based on the assumption of normal distribution. If this assumption does not hold, an extended procedure for the calculation would be necessary. The bootstrap approach could be used for that. It is not based on a theoretical distribution model, but uses the empirical distribution of the data for the estimation of the interesting parameters. A detailed formulation of the approach shall not be given since the assumption of the normal distribution (at least as an approximate distribution) can be justified by the Central Limit Theorem. Furthermore, the use of the bootstrap approach may inflate the statistical estimation error.

B 7 Residual analyses

Almost all adjustment methods discussed in this report are based on several statistical estimation methods. For the assessment of these methods the residuals, i.e. the differences r_t between measurement and estimated value, can be used. Under optimal conditions the variance of the residuals is constant, there is no autocorrelation, and there is no trend or a break in the structure.

The aim of the investigation presented is to elaborate an adjustment method which is well performing under very different conditions, that is to say, with sharply divergent time series, for different rivers and different substances. Therefore the residual analysis serves to understand the differences between the methods and to identify inadequate models. However, the assessment of the methods is based on the adjusted loads, and robust and simple methods are preferred even if the fit of the statistical model is not optimal. The effects of model deviations on the adjusted annual load is often quite small.

The following techniques for the analyses of residuals may be applied: Outliers can be explored by comparing the series of measured concentrations, the series of residuals and the series of the runoff. A graphical presentation of the residuals against the corresponding estimates allows an examination of heteroscedasticity. A graphical presentation of the residuals against the runoff allows an examination of the runoff effect. The histogram of the residuals allows the examination of the distribution assumptions, and the correlogram of the residuals and the calculation of the Durbin-Watson-statistics allow an evaluation of serial dependencies. Cross correlations between the residual series and the series of the runoff allow an assessment of the effect of lagged runoff.

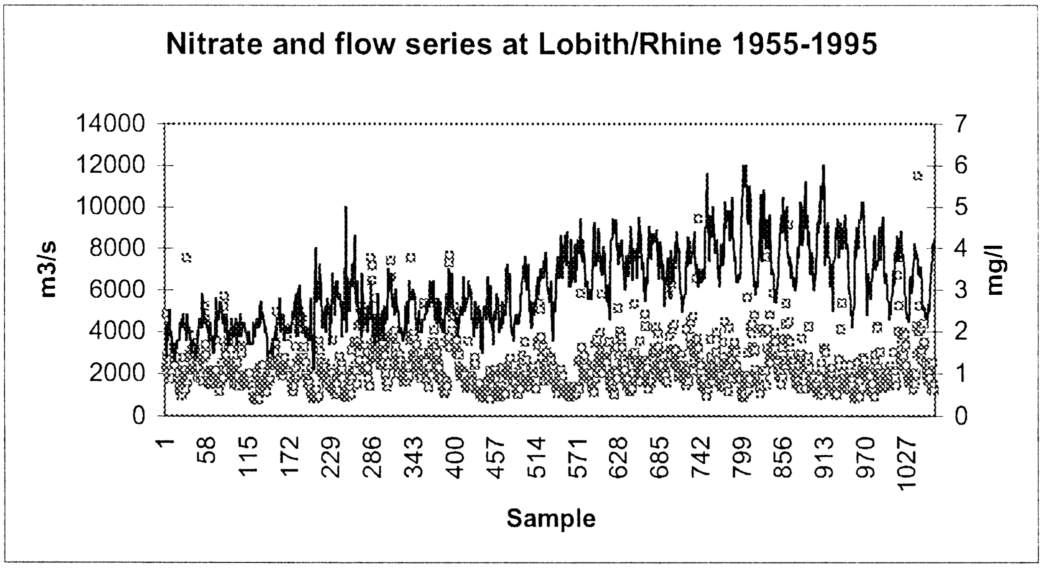
A numerical comparison between estimation methods can be obtained with the residual standard deviation s_{Res}, the percentage of the variance explained and with a modified AIC criterion:.

$$AIC = \ln s_{\mathrm{Res}}^2 + 2\frac{df}{N},$$

where df denotes the trace of the estimation matrix (smoother matrix). For locally calculated estimators df denotes the arithmetic mean of all locally calculated estimation matrices, and N denotes the corresponding window length.

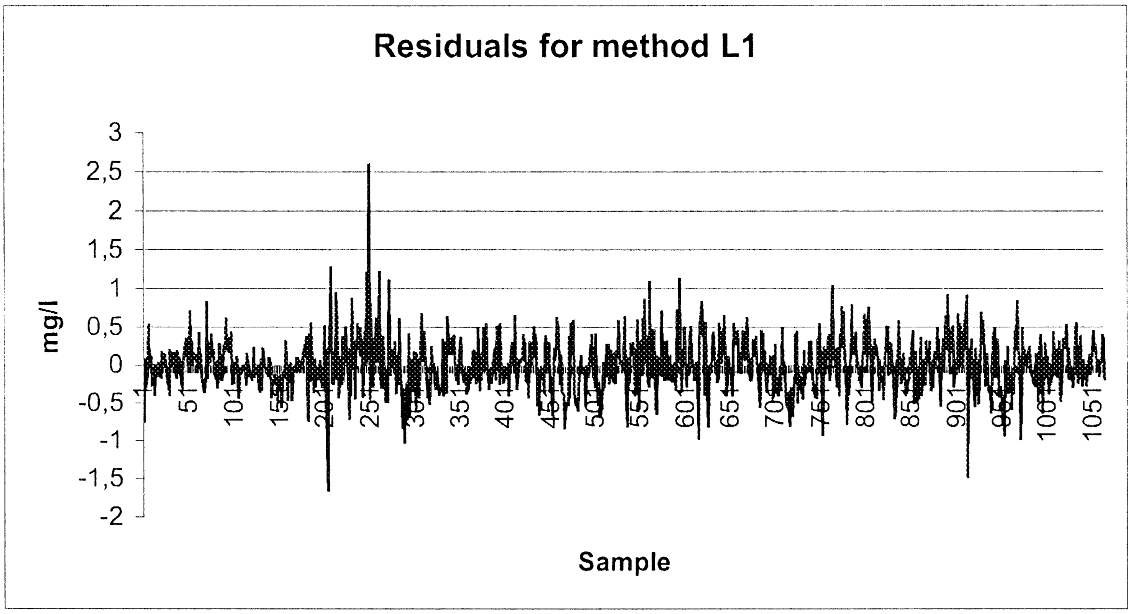
In the following, a residual analysis is presented for NO_3-N at Lobith using the methods L1 and H. Fig.B 7.1 contains NO_3-N concentrations (solid line) 1955-1995 at Lobith/Rhine and the corresponding runoff series (circles).

Figure B7.1



Considerable seasonality is to be seen in the series of the measured concentration. Fig.B7.2 contains a plot of the residuals obtained by method L1.

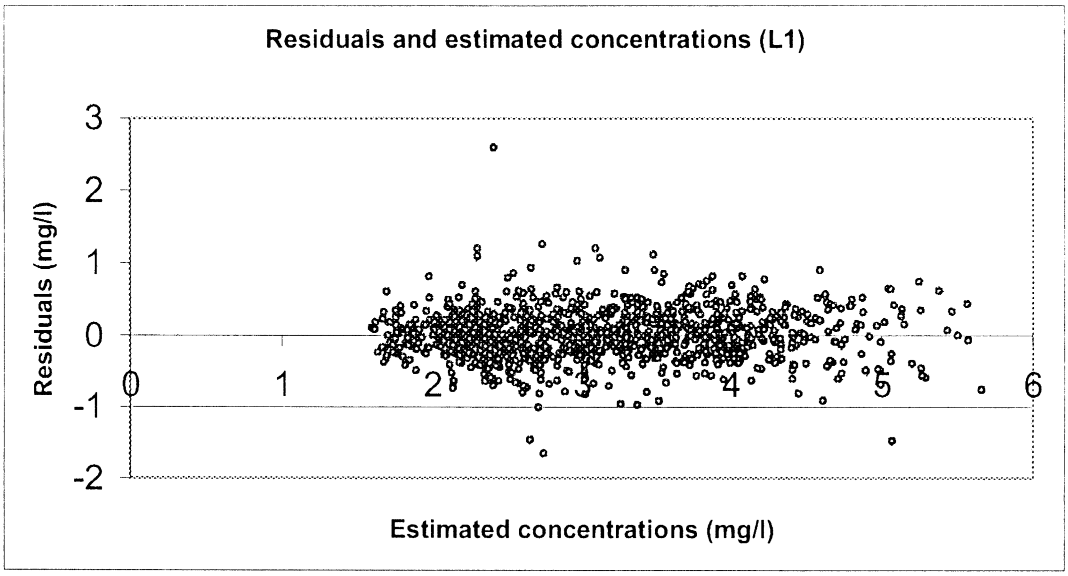
Figure B7.2



Apart from a few exceptions the deviations between measurement and model are below 1 mg/l. A model fit for the concentration series based on method L1 explains 86,6% of the variance, and the residual standard deviation is 0.35 mg/l. The indicator for the model fit AIC can be calculated AIC= –2.04.

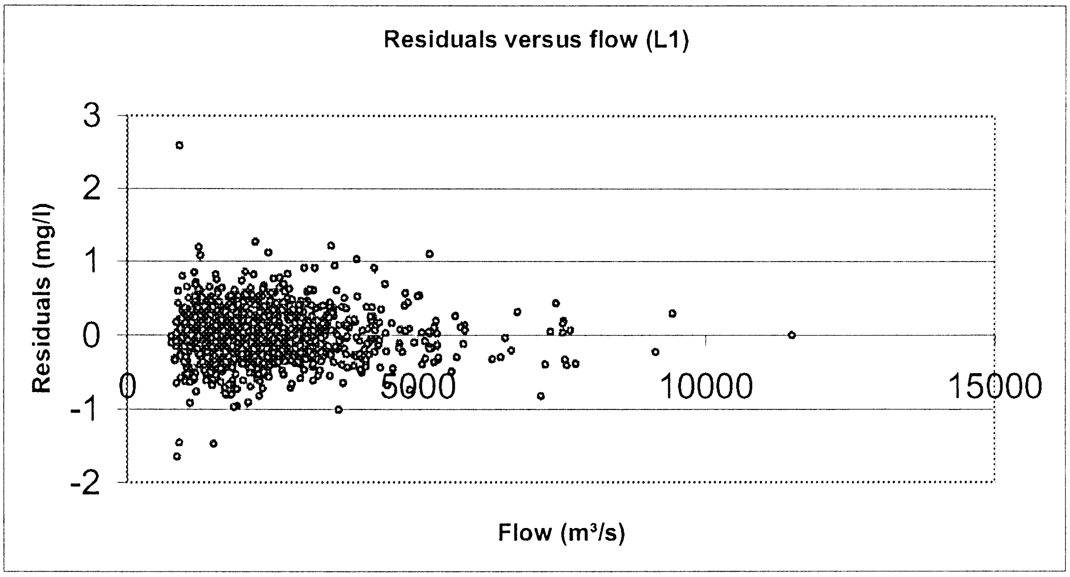
For an examination of heteroscedasticity the residuals are plotted against the estimated concentrations. A clear dependency between concentration level and variability cannot be detected.

Figure B 7.3



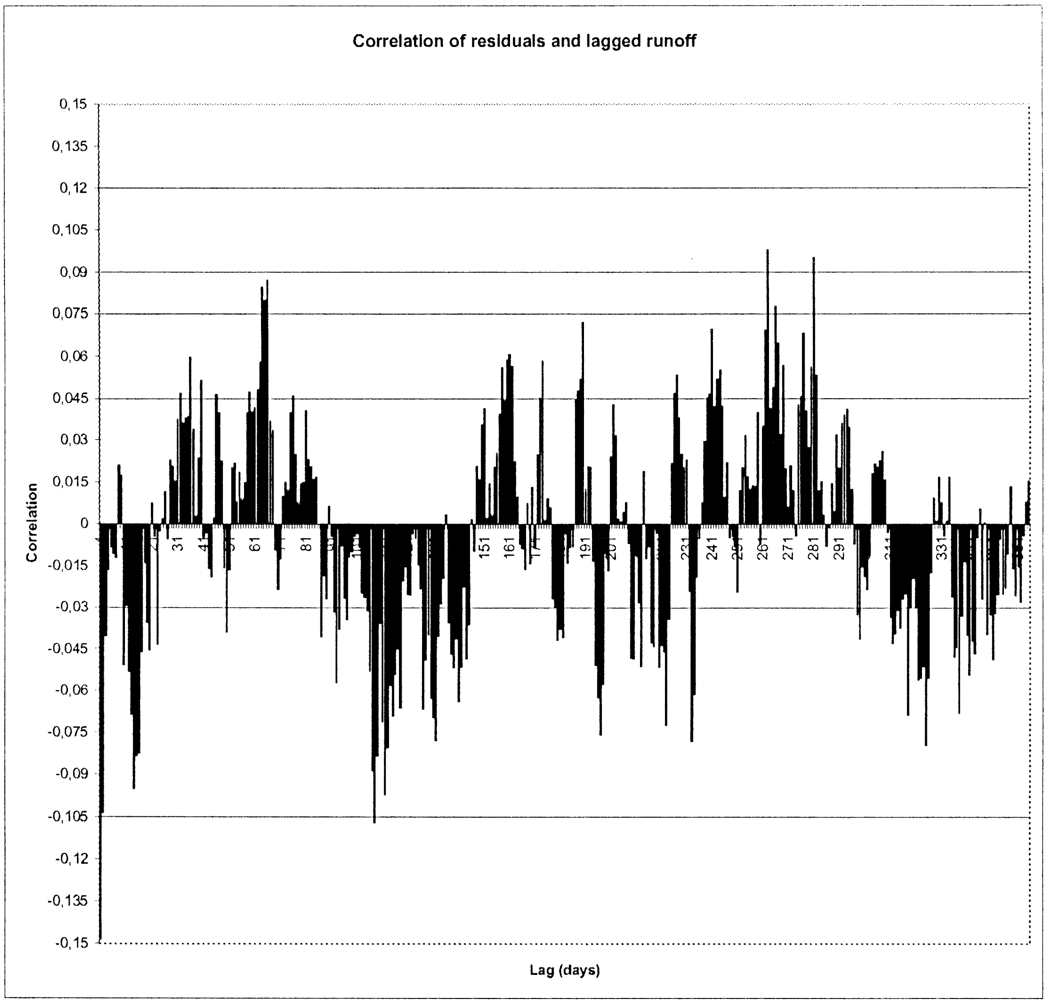
For an examination of the linearity of the LQ function the residuals are plotted against the runoff. No systematic dependency can be detected.

Figure B 7.4



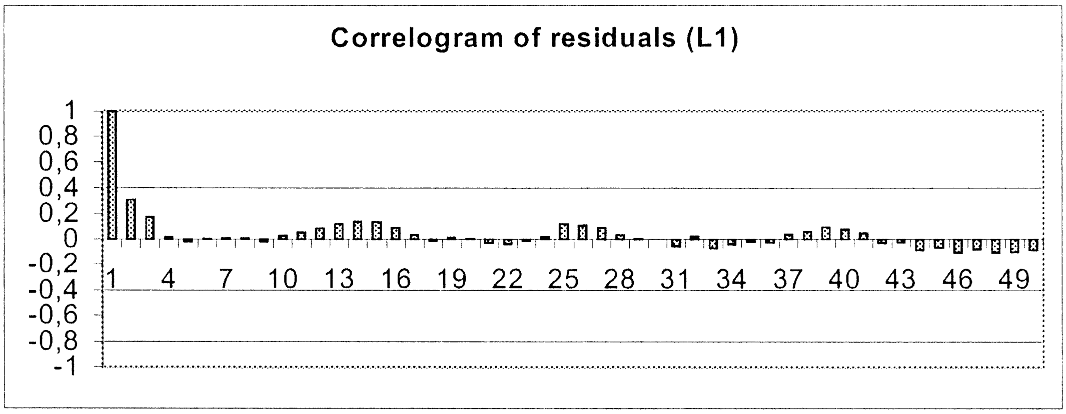
In order to assess the influence of lagged runoff, the correlation between the series of residuals and lagged runoff are calculated, but no clear dependency can be detected (Fig. B 7.5)

Figure B 7.5



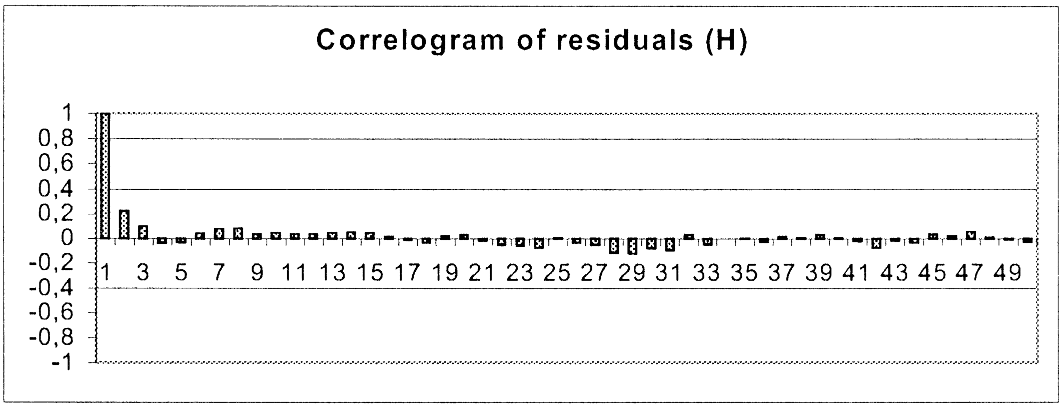
There is some autocorrelation in the series of the residuals, the Durbin-Watson statistics is 1.37 and the first order autocorrelation equals 0.31. The correlogram is contained in Fig. B 7.6.

Figure B 7.6



Apparently this is not a white-noise process and therefore it can be concluded that method L1 does not allow an optimal fit of the data. The fit could be improved by a time window of 5 instead of 7 years, or by use of method H. With method H 88.6% of the variance can be explained, and the corresponding residual standard deviation is 0.32 mg/l. The correlogram is given in Fig. B 7.7 and the Durbin-Watson statistic is 1.55. The AIC indicator for method H can be computed AIC=-2.13, i.e. this criterion prefers method H.

Figure B 7.7



Apart from slight first order autocorrelation (0.22, Durbin-Watson-statistics = 1.55) there is no remarkable autocorrelaton any more. Further improvement of the model fit could be achieved by

- reducing the window length,
- increasing the number of degrees of freedom,
- increasing the order of trend and season.

However, regarding the annual adjusted loads the differences between these methods can be neglected. The averaged relative deviation between these loads is 0.3%, whereas the averaged deviation to the load calculated with the OSPAR-formula is about 15%, i.e. 50 times higher. Similar conclusion can be obtained with other methods and other parameters.

B 8 Selection of an adjustment method

For the selection of an adjustment method it should be noted that the adjustment is not a straightforward mathematical correction method which deals with reach parameter in the same way. It may vary for every parameter and different time series. Temporal effects and seasonality have to be accounted for, and therefore the adjustment parameter have to be estimated using appropriate statistical estimation methods. In the investigation presented several estimation methods were implemented and tested, and it turned out that the differences of the resulting adjusted loads were relatively small, but the differences with regard to the fit of the statistical model were relatively large, i.e. the variation of the residuals was quite different for different methods.

It is principally not possible to determine a model which is generally optimal and which guarantees uncorrelated and normally distributed residuals which are homoscedastic. Another difficulty arises from single floods which may affect the load considerably and which complicate the calculation of the CQ function. Finally it should be noted that the dependency of the CQ function on the lagged runoff may lead to considerable over or under-adjustment. This may cause further complication and reduction of trend sensitivity.

For some parameters the model fit was not quite satisfying. This refers to violations of statistical model assumptions. Apparently the model fit for Pb was complicated by outliers and strong heteroscedasticity. These model violations may increase the estimation error. Alternatively one could use statistical models based on logarithmic concentrations, but then the model structure would not be additive any more (which was a precondition of the investigations). Another possibility is the development of a dynamic TBS model (Transform Both Sides; Carroll/Ruppert [1988]), but this is out of the scope of the project.

In order to account for the parameter-specific statistical distributions a parameter-specific model fit is necessary. Several indicators for the assessment of the model fit are available, as described in section B 7. A protocol for the selection of the method specifically for each parameter could be as follows:

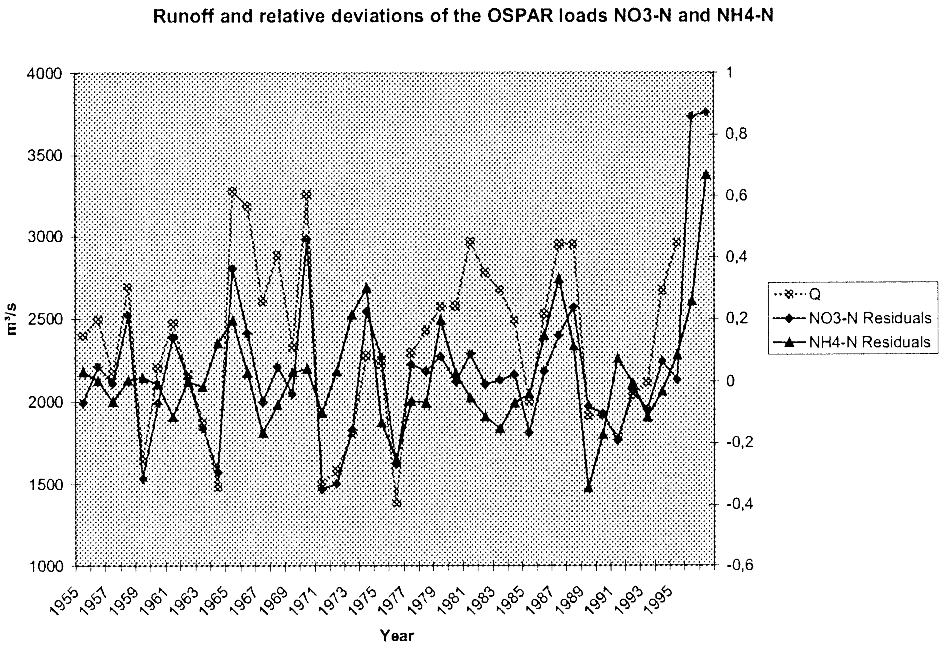
1. Apply method L1
2. Examine the residuals with regard to serial correlation using the test of Durbin and Watson, and apply method H in case of strong model deviations.
3. Examine the relation between runoff and residuals. In case of strong non-linearity a non-linear component should be taken into account (method L5).
4. Check correlation between residuals and lagged runoff and incorporate the lagged runoff if necessary (method L2).

If the methods L2, L5 or H do not achieve a satisfying fit, the model could be extended by further variables. Loglinear models could be another option in case of strong heteroscedasticity. In case of strong serial correlation the season term could be extended by components of higher order, the temporal trend term could be extended by a quadratic component or the method could be applied using a window of reduced length.

B 9 Interpretation of the correlation between runoff and the residuals of the OSPAR load

The very different results for different parameters and different rivers refer to the fact that the dependency between OSPAR load and runoff can be very different as well. A crude approximation can be obtained by the correlation coefficient ρ between the annual runoff and the relative deviations of the OSPAR load from the corresponding LOESS smoother. Fig. B 9.1 contains the latter and the runoff for NH_4-N and NO_3-N for Lobith. Apparently there is high correlation for the nitrate load, whereas the correlation for NH_4-N is low, especially in the years before 1970.

Figure B 9.1



For NH_4-N the correlation coefficient can be computed 26%, whereas for NO_3-N the corresponding value equals 86%. Assuming a simple linear model for for the relative deviations of the OSPAR load and the runoff, the percentage of the variance which cannot be explained by the runoff can be computed $1-\rho^2$. For NH_4-N one obtains $(1-0,26^2)=93\%$ and for NO_3-N $(1-0,86^2)=26\%$. For NH_4-N the incorporation of the runoff reduces the standard deviation by $1-\sqrt{1-\rho^2}=1-\sqrt{1-0,26^2}=3,4\%$, whereas for NO_3-N a reduction of 49% seems possible. Therefore $\sqrt{1-\rho^2}$ can be interpreted like the quotient S_{Ratio}. However $\sqrt{1-\rho^2}$ is based on annual data only, and therefore it can be supposed that the adjustment concept based on single measurements will allow smaller values for S_{Ratio} (depending however on the method applied). Apparently there is some relation between $\sqrt{1-\rho^2}$ and S_{Ratio}, and therefore $\sqrt{1-\rho^2}$ can be used as crude measure for the advantages of an adjustment.

Because of the considerable computational effort an adjustment is recommended only if $\sqrt{1-\rho^2}$ is below 0.9, i.e. if the standard deviation can be reduced by at least 10%. According to this rule an NH_4-N adjustment for Herbrum would be recommended, but not for Lobith.

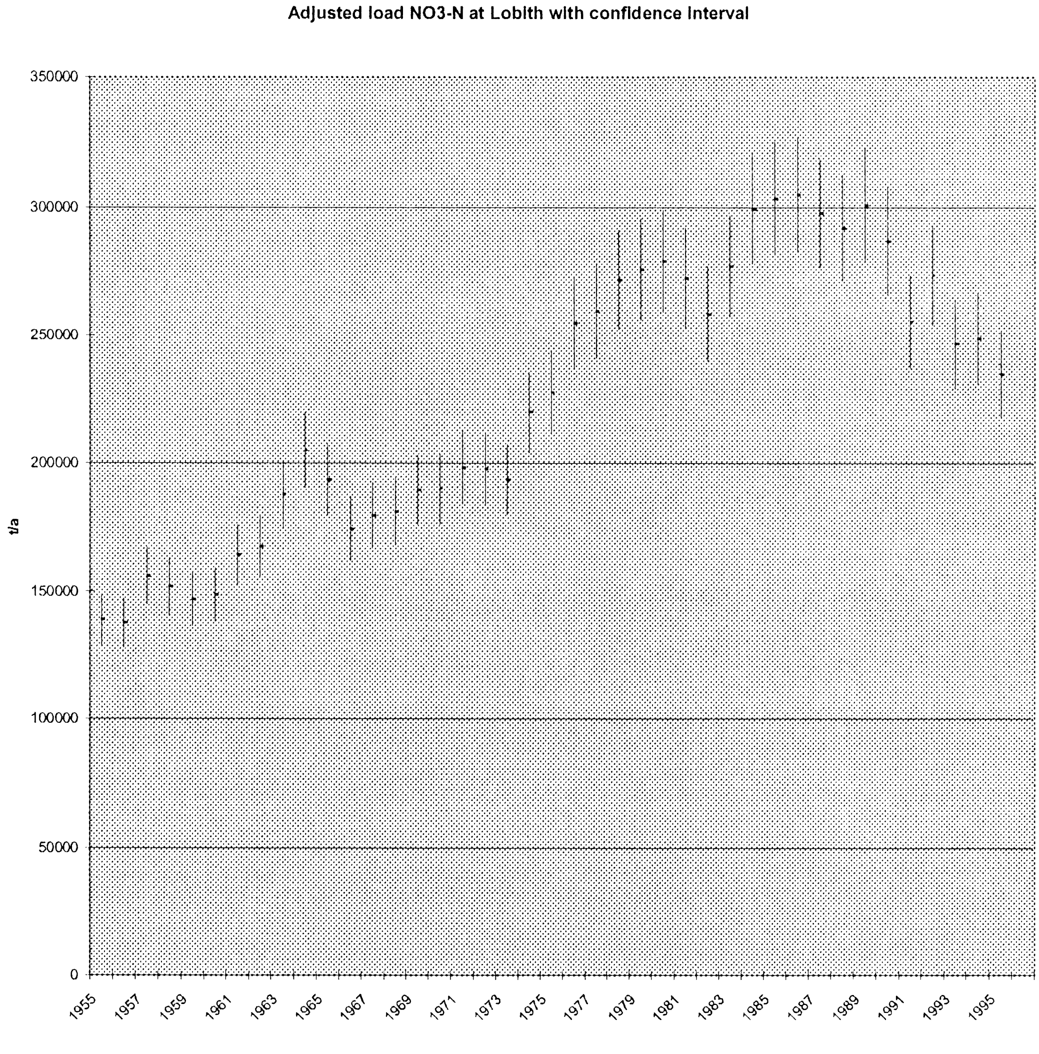
B 10 Confidence intervals for adjusted annual loads

Adjustment of annual loads aims primarily to improve the trend sensitivity. However, adjusted loads can also be used to assess direct effects and anthropogenic fluctuations. This appears meaningful if the random variations of the adjusted loads are not too large. Therefore a confidence interval for the adjusted loads would be helpful in order to assess erratic or rapid changes in anthropogenic inputs. Basics of such a calculation are described in chapter B 5. The calculation of the confidence interval should account for the serial correlation of the residuals since even small serial correlation may inflate the estimation error.

Fig. B 10.1 contains approximate confidence intervals for the adjusted nitrate load at Lobith. Apparently in 1973-1976 there was a rapid increase of the load. This cannot explained by random effects since for these years the confidence intervals do not overlap.[1]

[1] From a pure statistical point of view a significant change can be stated if the difference between subsequent annual loads exceeds the length of the confidence interval divided by $\sqrt{2}$. However the problem of multiple testing should be accounted for, and an additional correction of the critical values would be necessary. Disregarding these problems it it recommended to state a significant change if the confidence intervals do not overlap.

Figure B 10.1


Adjusted load NO3-N at Lobith with confidence interval
t/a
350000
300000
250000
200000
150000
100000
50000
0
1955
1957
1959
1961
1963
1965
1967
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1977
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1995

Trend analysis and adjustment of river loads

RTrend

Software program for trend analysis and adjustment of load data

Documentation

RTrend

Documentation

May 2001

Version: 2.0.0.18

For WINDOWS 9x and WINDOWS NT

Software development: quo data GmbH

Programmer: Dipl.-Ing. Norbert Schick

Dipl.-Phys. Andre Fränzel

Dipl.-Math. Dirk Anke

C 1. Table of contents

C 2. Basics

C 2.1. Introduction

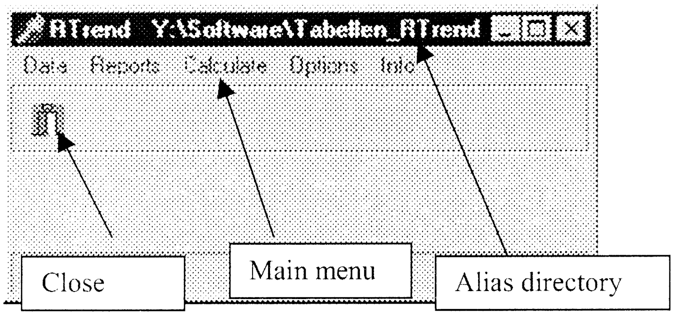
The program RTrend is intended for the statistical analysis of riverine loads. Data are stored in a data base in the format PARADOX 7.0. The data base is derived from the NILU data base developed by Ter Krognes. Its 23 tables permit the flexible and easily expandable storage of the most diverse specification, which is relevant for an analysis. The structure of the data base and the fields of the individual tables are shown in Annex 1.

The program is written in the language DELPHI version 4.02 with the modules TeeChart version 4.1 pro and QuickReport version 3.05. The structure of the program is represented in Annex 2. Language of the program is English. Individual labels in other languages are due to the language of the operating system used.

A paradox data base consists of one or more files (tables) contained in a common directory. Access to the database is managed via an alias name, which refers to the directory of the database. The program RTrend uses the alias name "trend" for the access to its data base. After the installation of RTrend a sub directory *Tables* is created. It can be modified via the *data* menu.

The program contains the following functions:

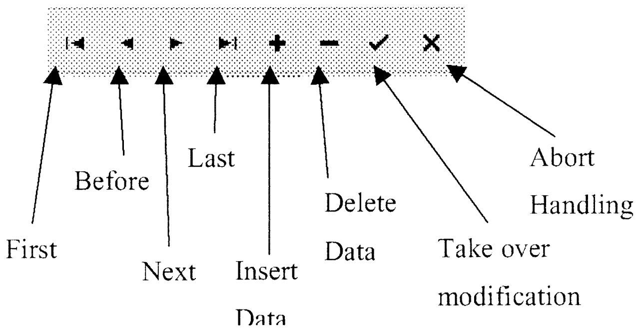
Menu Data: Input and modification of data as well as import of data from different formats.
Menu Reports: Display of data in tables and diagrams (several parameters for a station, one parameter for several stations etc.).
Menu Calculate: Preparation of data for the adjustment, calculation of the adjustment, aggregation and trend analysis.
Menu Option: Settings, e.g. the formats of values.
Menu Info: Info Dialog.



Picture 1: Main form

C 2.2. Database handling

The input and modification of data been made into the data base by the appropriate windows, generally thereby the handling is controlled via a navigation bar:

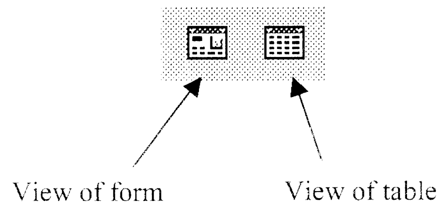


Picture 2: Navigation bar for data base tables

If some operation with the navigator bar cannot be executed, the pertinent button is deactivated (represented grey). Each input and modification of a data record have to be confirmed upon clicking the *accept* button. This saves the data record. A storage of the data record takes place automatically if an input or a modification to a new data record is made.

Be careful: A modification of the data cannot be cancelled after storage!

The data can be displayed either in forms or in tables. Click on the appropriate button to select the required mode:



Start date

In many forms and tables the field start date is available. Enter the date which refers to the information in the form. Purpose of the field is a history function, which is however not yet implemented. Therefore the date is currently without meaning.

Dates instructions

Dates are to be entered in a four-digit format, in order to avoid the "millennium bug" problem (01.01.99 corresponds to 01.01.2099!).

Table formats

The column width in a table can be modified as under EXCEL. The mouse pointer must be positioned in the column headline on the vertical separator line to be modified. Then the pointer take on the shape of a double arrow. After pressing the left mouse button the column width can be modified by moving the mouse pointer.

In the tables of some windows it is possible to rearrange the order of columns. Place the mouse pointer on the respective column heading and click on the left mouse button in order to activate the menu for arranging the columns.

C 3. Menu structure

C 3.1. Menu Data

C 3.1.1. Data / Edit Main tables

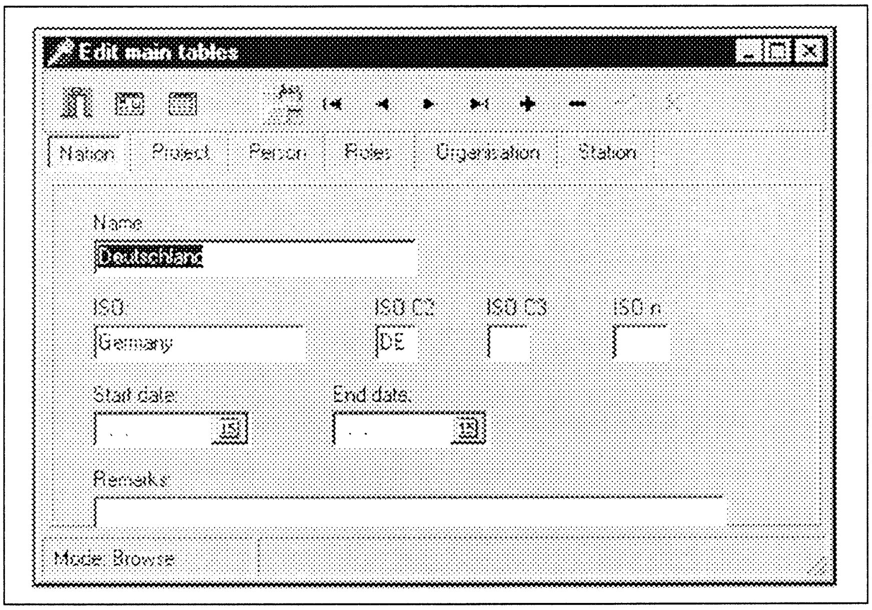
In the menu *Edit Main tables* the basic data can be entered and modified. Data are assigned to the following categories:

- *Nation*
- *Project*
- *Person*
- *Roles*
- *Organisation*
- *Station*

It is recommended to enter the data in the sequence given above., since e.g. station data cannot be entered without a nation and an organization. Modifications of the key fields afterwards should be avoided, and if it is unavoidable, a backup should be made before.

<u>Nation</u>

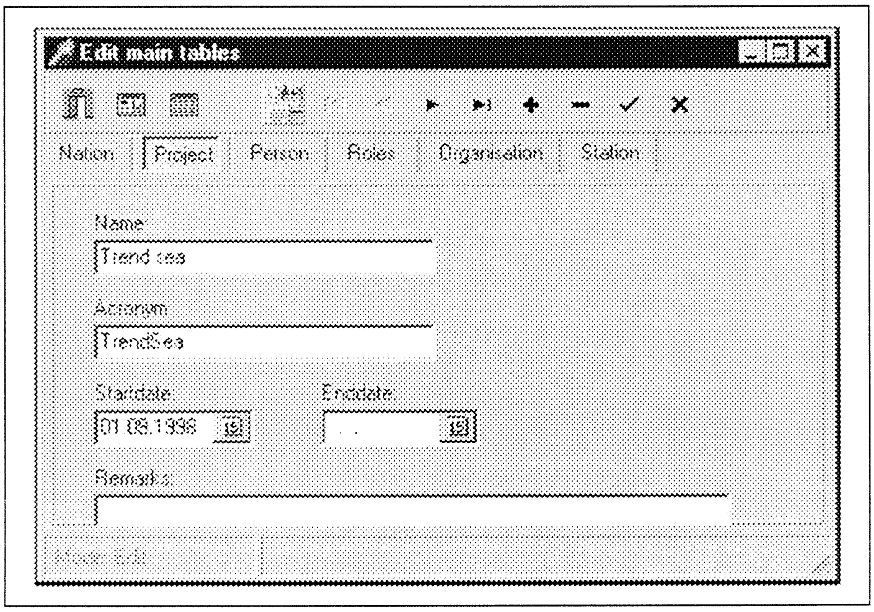
The menu *Nation* enables the input and modification of all data to a specific country, which are also necessary for a report. The ISO C2 - code is a key field and should afterwards not be changed. It is used as identifier in subordinated tables which are not automatically updated at present.



Picture 3: Form *Nation*

Project

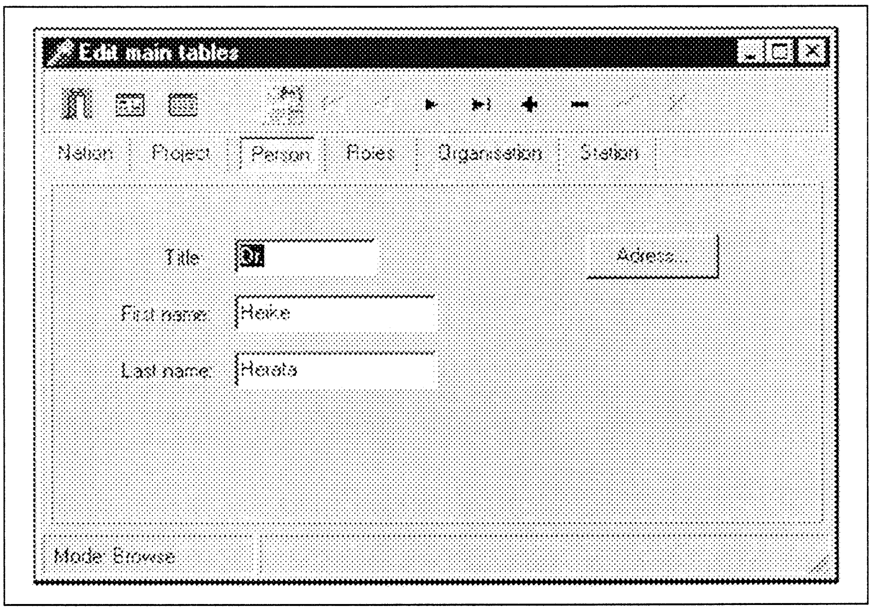
The data can be assigned to different projects by the menu *Project*. In order to allow an assignment of the data, at least one project should be registered. Key field is the field "Acronym".



Picture 4: Form *Project*

Person

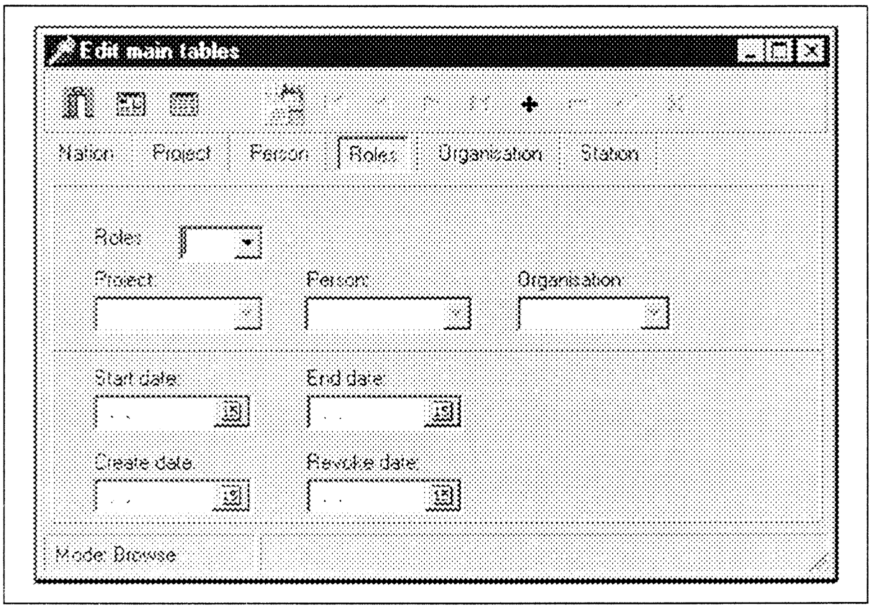
The menu *Person* contains personal data for the reporter, the responsible person, or the person to turn to. The persons registered can be assigned to organizations, stations and data sets. An internal key field is used, so that modifications of the data are possible.



Picture 5: Form *Person*

Roles

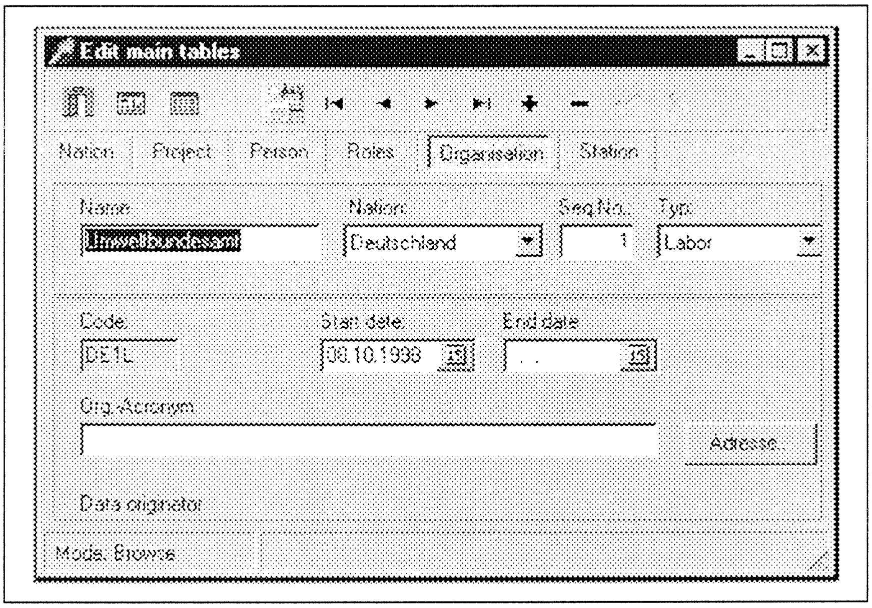
The menu *Roles* is not used at present. It is intended to use it in an extended version of the program for a description of functions of persons and organization within specific projects.



Picture 6: Form *Roles*

Organisation

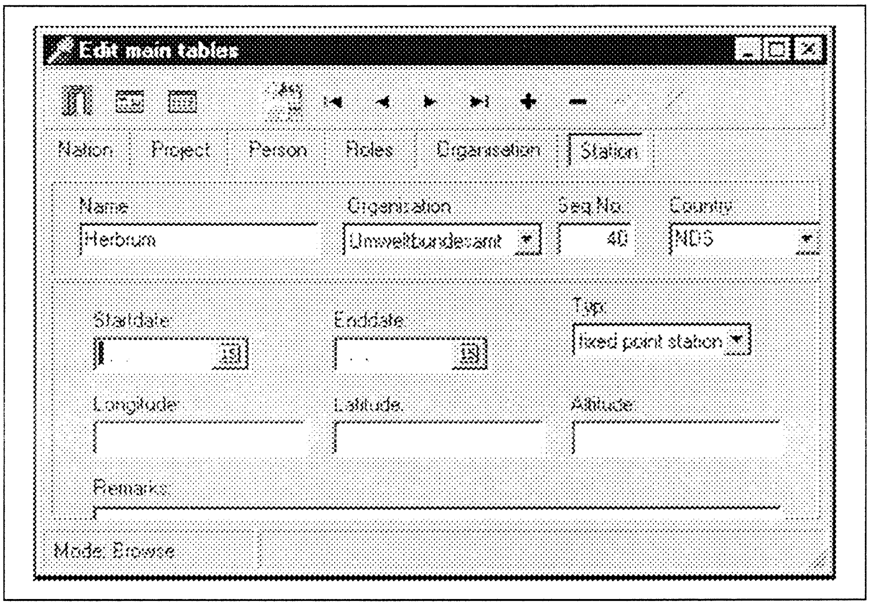
In the menu *Organisation* the input and modification of data for the body responsible for the national monitoring network takes place. The specification of the name, the nation, the sequence number (Seq. NO), the start date and the type is mandatory. The sequence number is a key field and should not be modified afterwards.



Picture 7: Form Organisation

Station

The menu *Station* allows to enter and to modify the basic data of the measurement stations. The name, the organisation, the sequence number and the start date are mandatory. A station code is formed automatically using the nation code (for example DE) and a sequence number (e.g. DE0001), which is used for the identification of the station in all tables. The station code cannot be modified by the user.



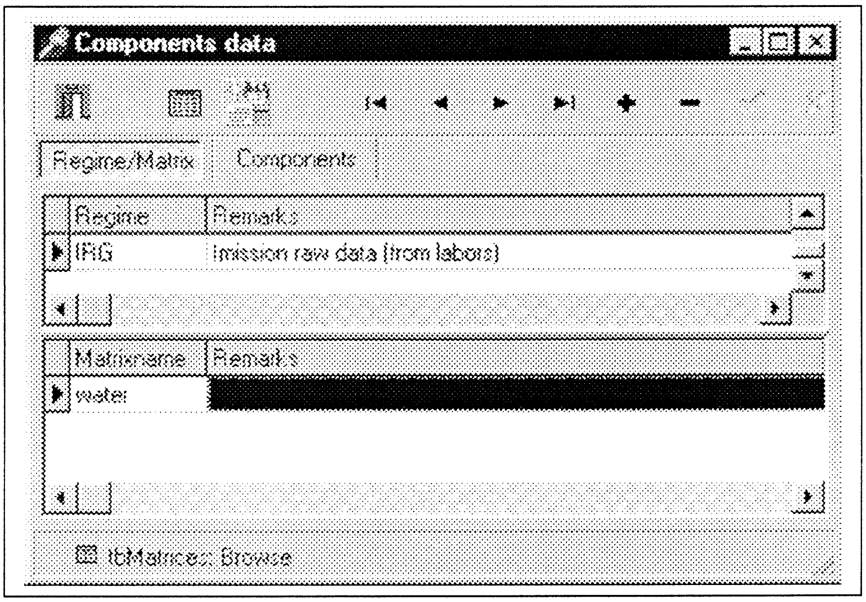
Picture 8: Form Station

C 3.1.2. Data / Components tables

In the menu *Components tables* the basic data referring to substances or other chemical parameters, the corresponding matrices and the type of data can be entered and modified. The data base contains the definitions of the NILU database. A modification or extension of these definitions is possible without problems.

<u>Regimes/matrices</u>

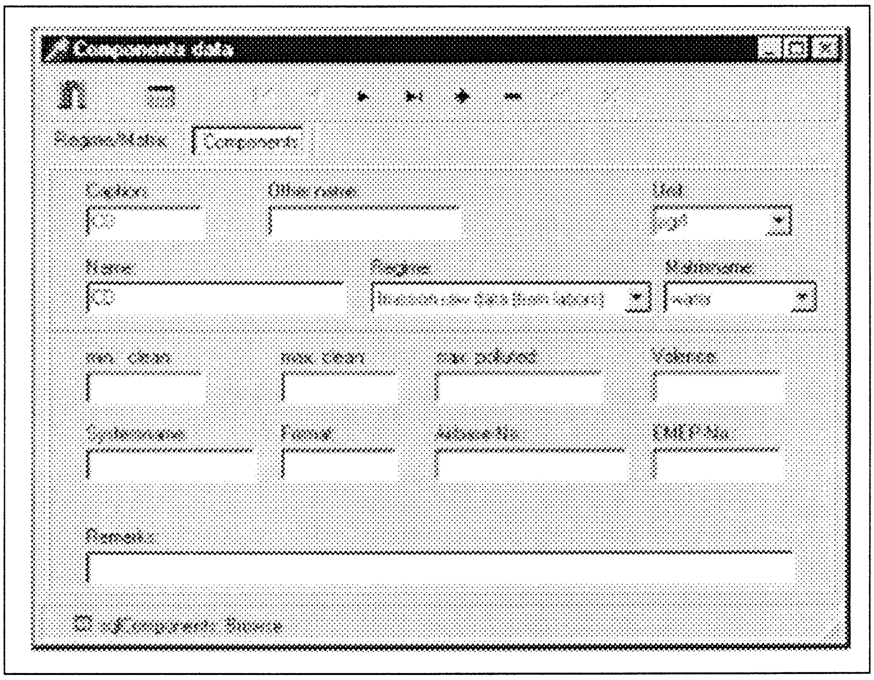
With a specification of regime and matrix the measured parameters can be assigned to different categories. The regime specifies the type of the data (immission value, emission values; measured, modelled...), whereas the matrix indicates the origin of the data (water, sediment...). The matrix name and the regime code are key fields.



Picture 9: Form *Components data*

Components

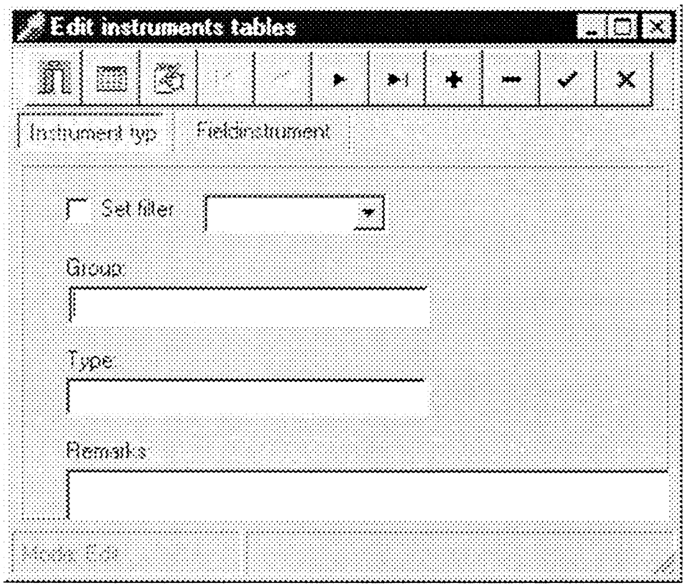
A component is determined uniquely by the name of the parameter measured, the matrix name, and the regime. Therefore these fields are mandatory. A specification of the "caption"-field is necessary because it is needed for the description of the components in diagrams and tables. The other fields are optional, although it is recommended to enter the measurement unit.



Picture 10: Form Components

C 3.1.3. Data / Instruments tables

The menu *Instrument tables* allows to enter a description of the instrument classification (instrument type) and a description of the field instruments. Firstly the instrument types have to be entered and then the field instruments can be described.



Picture 10: Form Instrument tables

C 3.1.4. Data / Datasets

Access to the measurement values measured in the database can be obtained by the menu *Datasets*. The measurement values are stored in different tables and separated with regard to the component. The table names correspond to the component names with an additional prefix "DV_".

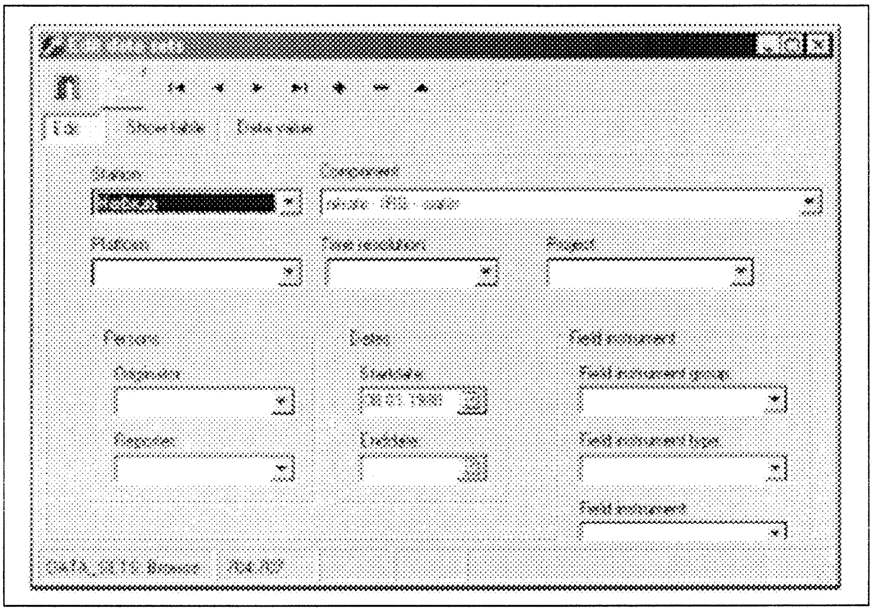
In order to avoid unintended changes in the data sets, editing is only possible by clicking the edit button in the database navigator. The function key F9 switches into a permanent edit mode. This procedure exclusively applies to the menu Datasets.

There are three forms available:

Edit displays the dataset selected. Can be used to enter basic of the dataset.

Show table displays the table of names and descriptions of the datasets.

Data value displays the measurement data for the selected dataset.



Picture 11: Form Edit

The forms *Show table* and *Data value* are omitted.

C 3.1.5. Import EXCEL file as CSV

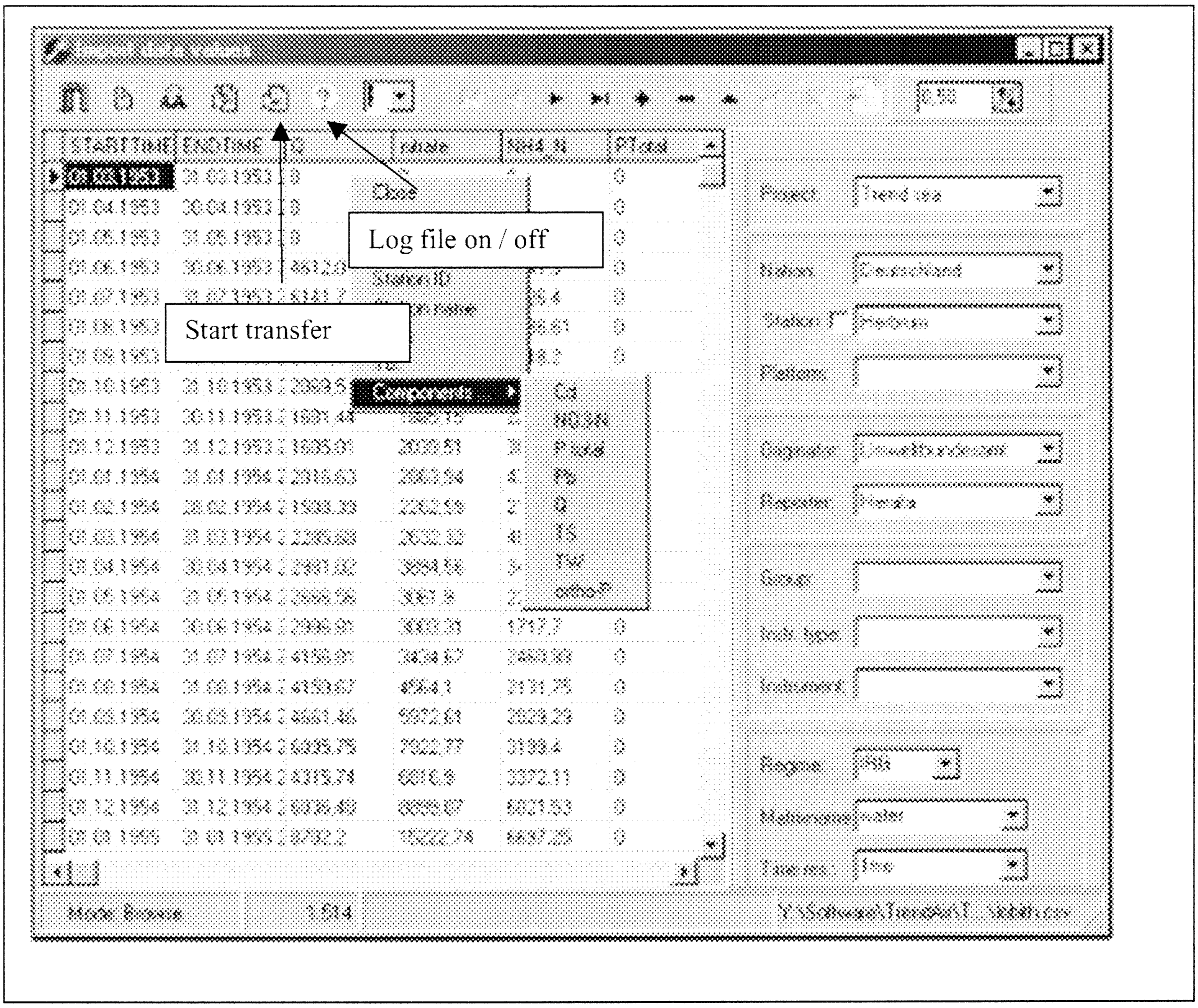
For the import of measurement values a flexible import module is available. The import of measurement data is based on an ASCII file (CSV), the values of which are sorted in lines. The values within one line are separated by ";" or by ",".Such a file can be produced easily in Excel. As type of file thereby the CSV format is to be selected.

After the file has been opened, the table will automatically be displayed in the menu *Import*. No data is entered yet in the table at this point. Start with the selection of the regime and the matrix, because these data affect the further import processing. Now verify the structure of the table and assign the names and measurement values to the columns by clicking on the column headers and then choosing the desired field from the drop-down list box that opens. The available components are listed in the sub menu *Components*. If you discover erroneous entries in the table, you can correct them by activating the *Edit* mode.

Data can only be imported, if there are values available for the field station ID (EB_SEQNO), starting time (DV_STARTTIME) and end time (DV_ENDTIME). If the field station ID is missing from the file, the name has to be entered in the respective field in the entry dialog box and the field next to this one be checked. This name will then apply to all records in this file. The others specifications which must be available, are

Project name	(field Project)
Instruments group	(field Group)
Instruments type	(field Instr. type)
Instruments name	(field Instrument)

It has to be noted that these selections determine the import dataset, i.e. the import data are transferred into the dataset with the same specification. Data with same project name, same station, same component but different instrument specification are written into different datasets. Then the statistical analyses will be performed separately for each dataset.



Picture 12: Import CSV-files

Before the data can be transferred into the database, all lines which contain not measurement values must be deleted (heading lines). Further it is to be noted that all modifications have only temporary character and will be not written back into the CSV file. Finally the substitution factor (default value=0.5) for the substitution of measurements is to be controlled. Measurements below the determination limit will be replaced by the product of the substitution factor and the determination limit. After you have checked the plausibility and correctness of the assignment of all table columns, start the transfer into the database by clicking the button *Start transfer*.

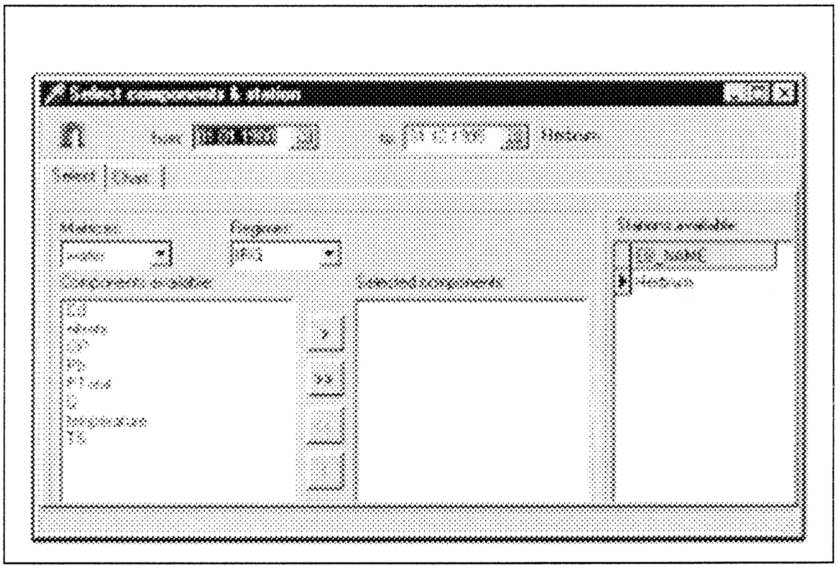
Now all measurement value are transferred to the database one after the other. All details on the changes in the database are recorded in a transfer protocol. This transfer protocol consists of an ASCII file (log file) and can be opened by clicking the button *Log file on / off*.

Afterwards the log file should be deleted (by clicking the button a second time).

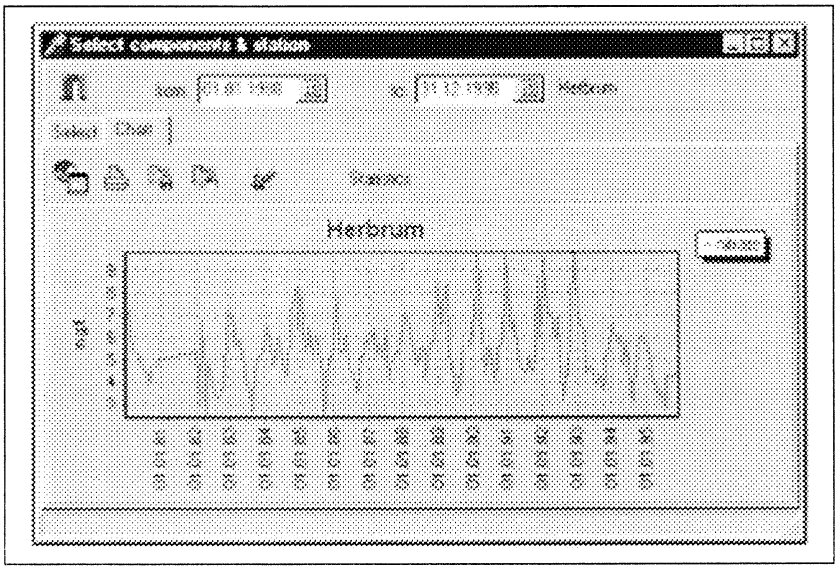
C 3.2. Menu Reports

C 3.2.1. Reports / Components

The menu *Reports / Components* allows the graphical representation of up to ten components for one station. The measurement data are plotted in a line diagram. All plotted components have to be assigned to the same regime and the same matrix. Furthermore a specification of a time interval of the measurement values is necessary. Click the button *Chart* to display the diagram.



Picture 13: Form Components – Select

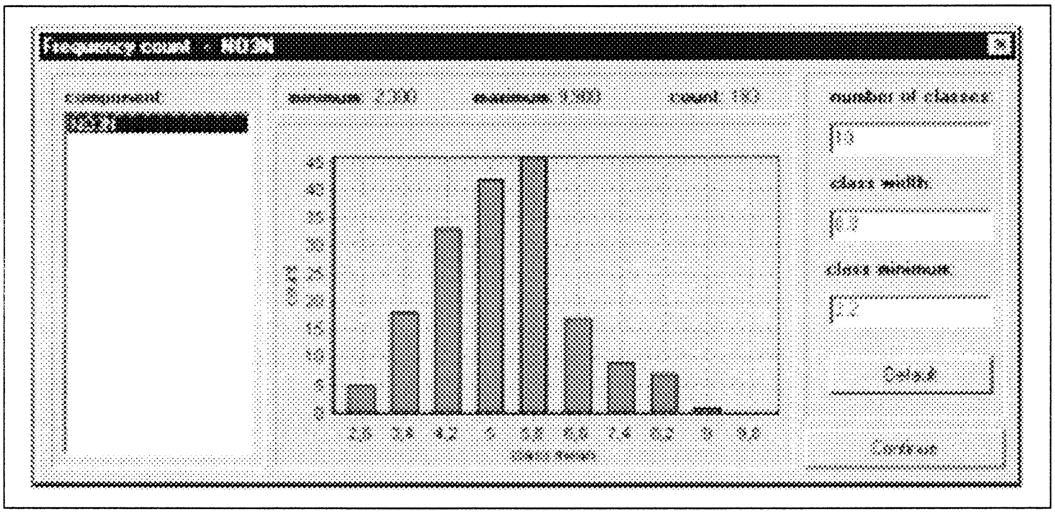


Picture 14: Form Components – Chart

The diagram can be printed, a WMF file can be created (after the Save as dialog has been completed) or copied into the clipboard. Please note that WMF files are not interpreted by all programs in the same way, so that under certain conditions some objects (titles, scales) may be distorted or displaced.

For a black-and-white output the colored representation can be suppressed with the button *Color print on/off*. Then it is recommended to activate the diagram editor and to edit the lines in an appropriate way. In case of problems with the printed output it is recommended to check the printer driver.

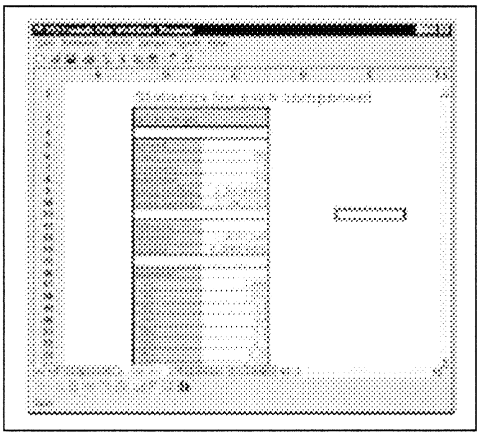
The button *Statistics* allows the calculation of the frequency distribution as well as important percentiles of the data selected. The partition of classes can be manually determined:



Picture 15: Histogram of the data selected.

Click the button *Continue* to create an Excel-conformal worksheet which contains the frequency distribution as well as the following descriptive characteristic values and the measured values itselves:

- Minimum
- Maximum
- Arithmetic mean
- Geometric mean, (the n^{th} root of the product of the n measurement values)
- Standard devation
- Relative standard deviation
- Percentiles for p=2%, 3%, 5%, 25%, 50%, 90%, 95%, 97%, 98%



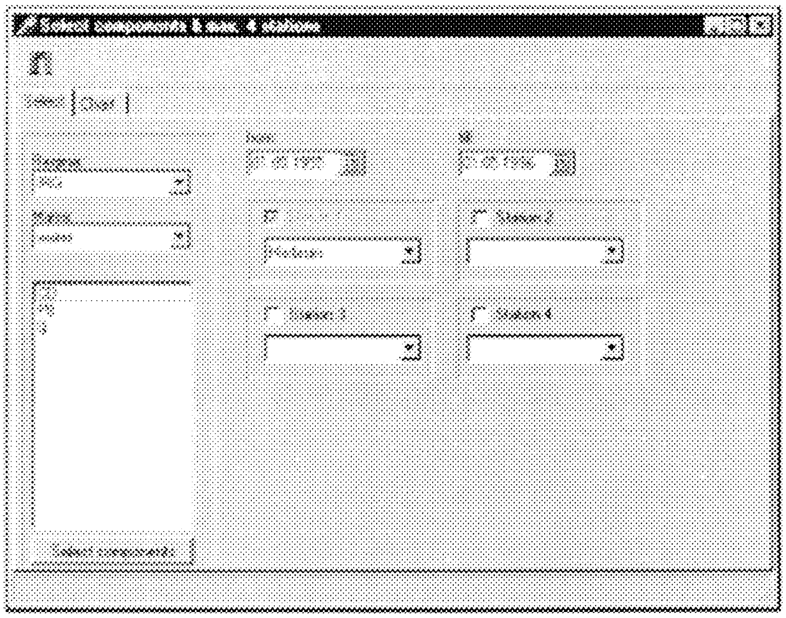
Picture 16: EXCEL-conformal worksheet

C 3.2.2. Reports / Stations

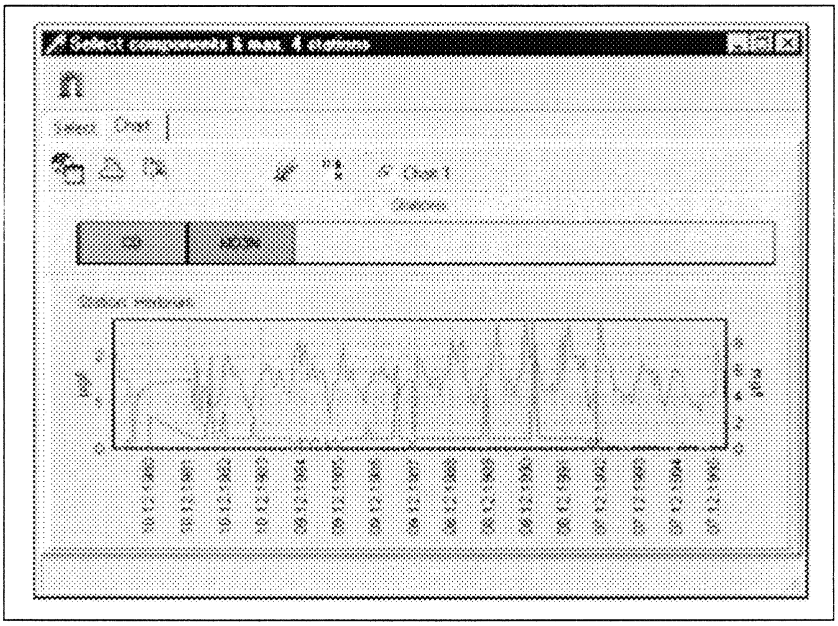
The menu *Stations* allows the graphical representation of the measurement results of up to ten stations for one component. Procedure and output is analogous to the menu Components .

C 3.2.3. Reports / Components & 4 stations

The menu *Report / Components and 4 stations* allows a combined chart of selected components of 1-4 different stations. Diagram 1 (station 1) is always activated.



Picture 17: Data selection for a combined chart of 1-4 stations



Picture 18: Diagram view

The diagrams can be activated by selecting the corresponding button.

C 3.3. Menu Calculate

The menu *Calculate* allows the preparation of raw data for the calculation of adjusted loads, the aggregation of adjusted and unadjusted loads and the analysis of trends. The preparation of raw data for the calculation of adjusted loads and the aggregation of unadjusted loads is controlled by the sub menu *Calculate / Make database*. In this menu a temporary database is created which includes the data necessary for adjustment and trend analysis. Adjustment, trend analysis and power analysis is controlled by the sub menu *Calculate / Adjustment*.

C 3.3.1. Calculate / Make database

The menu *Calculate / Make database* controls the selection of components, the time interval, the station and the temporal resolution. The components are classified as follows:

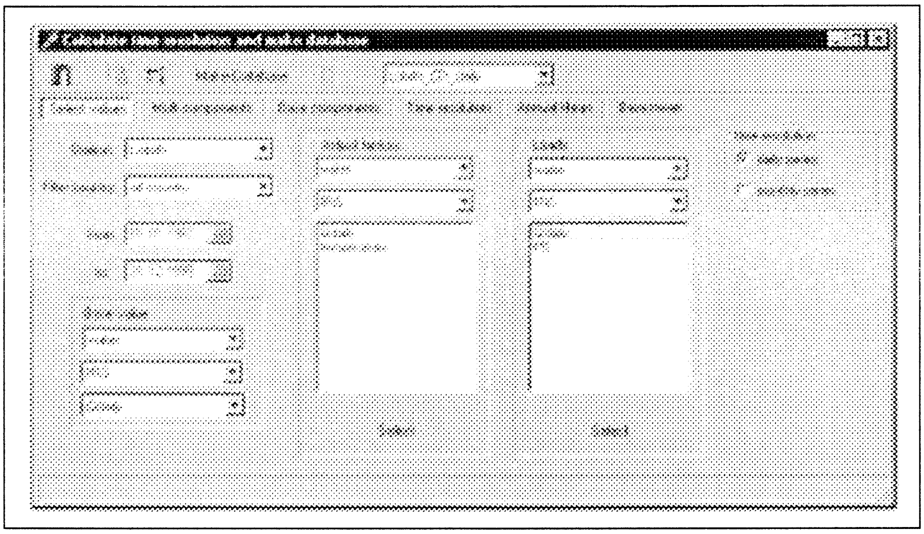
Base value: this is the runoff measured daily and denoted by Q.

Adjust factors: these are the factors required for the adjustment step, e.g. the runoff and the temperature.

Loads: these are the substances for the load calculation. The selection of several substances is possible, but it is strongly recommended to analyse one parameter at a time. For reasons of limited memory the residual analysis as performed for one parameter only.

Start and end time and the time resolution are needed to perform the calculations. Furthermore the *Base mean* has to be available in the database. This is the monthly long-term mean of the runoff. If some data are missing, an error message is created if the menu is opened or the station is changed.

After opening the menu the settings of the last session are entered automatically. If you want to activate another already available selection, open the drop-down list box on the toolbar and select one of the selections. It should be noted that the name of the selection is under control of the user. If you change the name of the station, the name of the selection should be adapted as well.



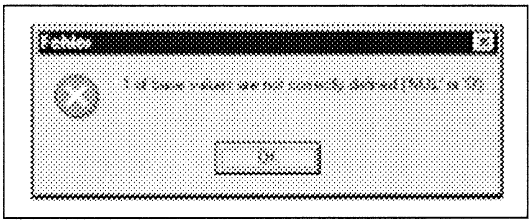
Picture 19: Selection menu for the preparation of data

After the selection of the base value, the adjustment factors and the load parameters press the button *Make Database* to perform the data preparation. The result of this process are three tables

- *Multi components*
- *Base components and*
- *Time resolution.*

which contain the results of the subsequent steps of data preparation. The table *Multi components* contains the raw measurement data which for the adjustment and the calculation of concentrations. In the table *Base components* the same data are assigned to the temporal structure of the base variable. The table *Time resolution* contains the final table, either on a daily basis or monthly aggregated.

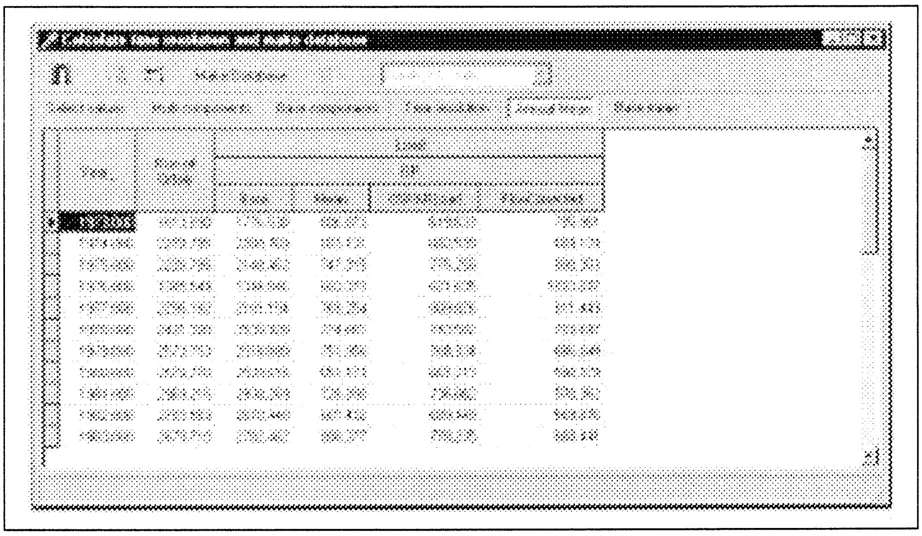
In case of missing flow data (base value or monthly long-term mean) the calculations may be wrong, and therefore a warning is created:



It should be noted that some adjustment methods are able to deal with missing values, but others not. The function *Compress* in the *Calculate / Adjustment* menu has to be used in that case.

If the calculations are finished, the results have to be saved using an appropriate file name. It is recommended to use meaningful names which allow an assignment to the respective station and the components included. In order to save the selection, press the command button *Save component*. If the calculation is repeated without saving the results, the previous data are not available any more. Files which are not required any more, can be deleted with the command button *Delete*.

Apart from the three tables *Multi components*, *Base components* and *Time resolution* there is a fourth table containing the annual aggregated loads. These can be displayed by clicking the button *Annual Mean*:

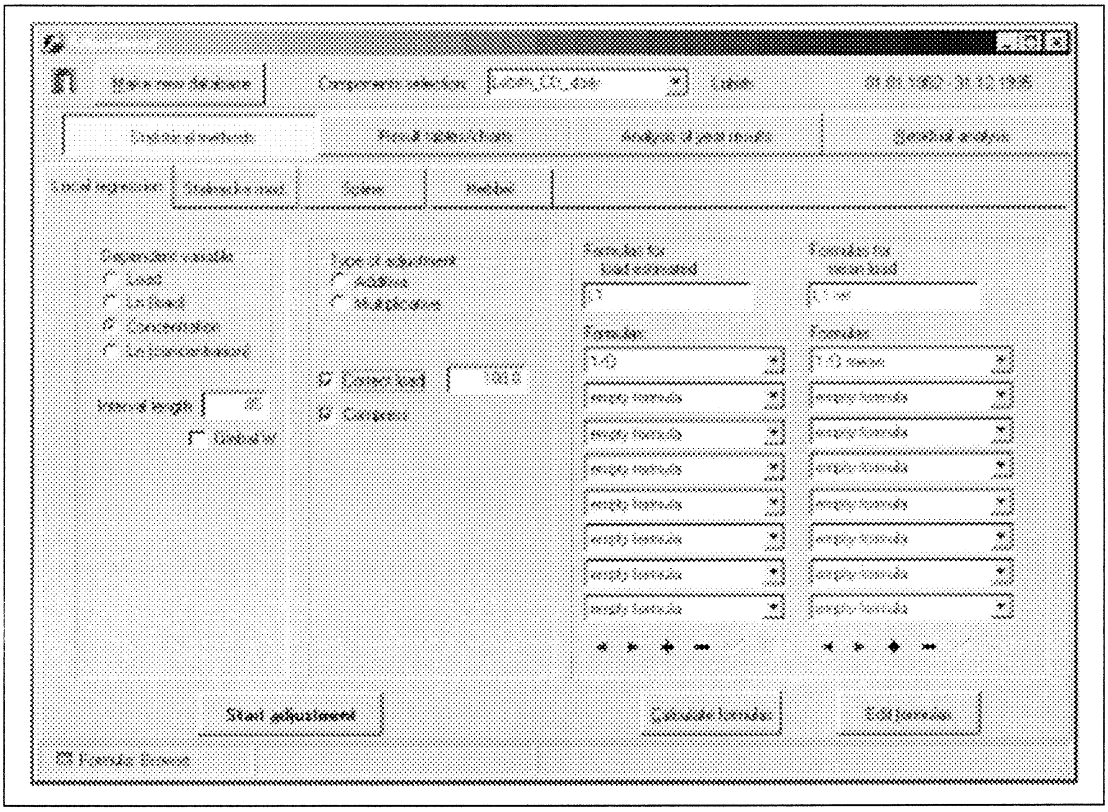


Picture 20: Annual mean table

In the second column of this table the average runoff for the respective year is entered. The third column contains the average runoff of those days of the year, where concentration measurements were carried out. The annual load is obtained by averaging the product of the concentration values with the flow values. It is put down in the column *Mean*, while the column *OSPARLoad* contains the load calculated according the OSPAR formula. This is the flow-weighted load. The last column contains the flow corrected load according to method A0. This is calculated on the basis of the long-term mean runoff.

C 3.3.2. *Calculate / Adjustment*

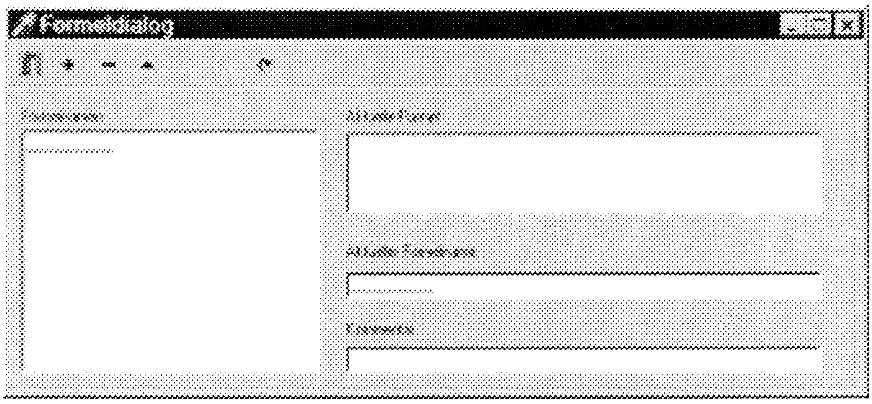
This menu controls the adjustment step and the trend analysis. Several procedures are available for the adjustment step. The menu looks as follows:



Picture 21: Selection of the adjustment method and the parameters for the adjustment

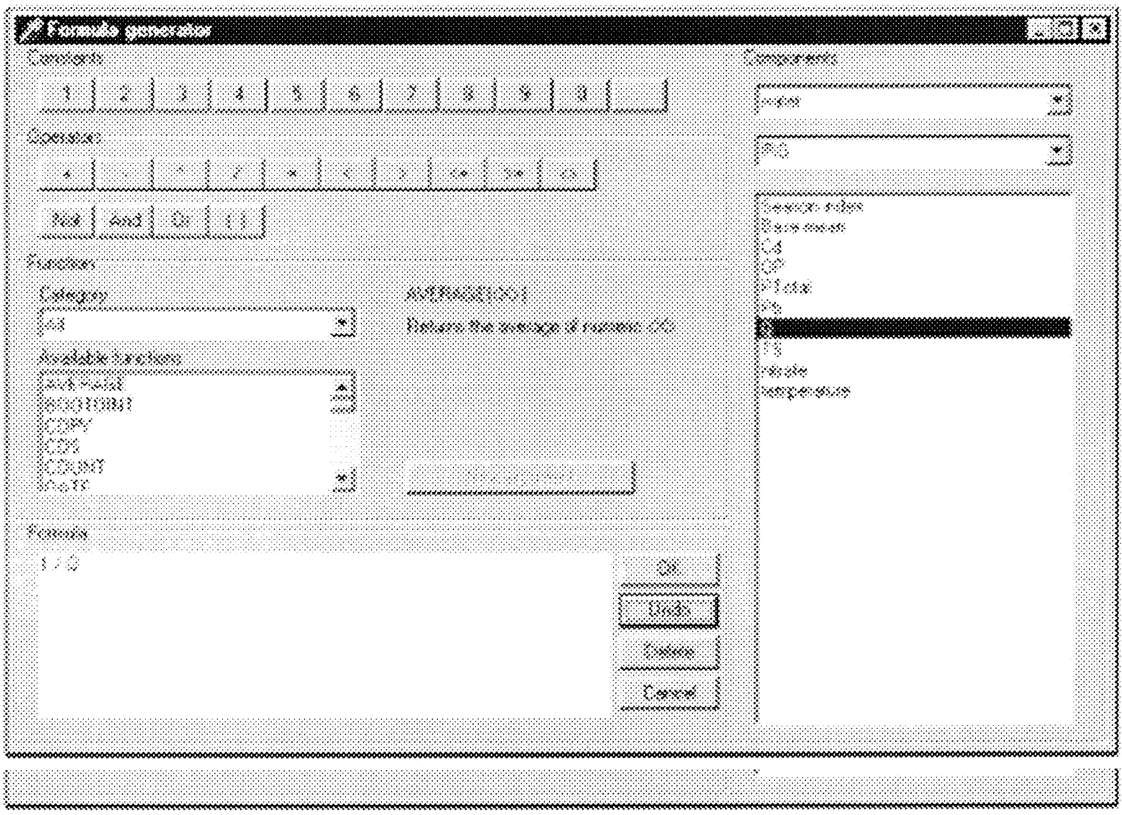
In the present case the menu page *Local regression* was activated. The *Local regression* page allows the calculation of the methods L1, L2, L3 and L4. The calculation procedures for the other methods are similar.

In preparation of the adjustment step the formulas for the adjustment factors have to be entered. Click on the button *Edit formulas* to get an overview of the formulas available:



Picture 22: Edit formulas

The formulas are saved in the data base and can be added, deleted and edited. Press the command button + to open the *formula generator*.



Picture 23. Formula generator

The *formula generator* allows the generation of formulas based on the adjustment factors and load components defined in the menu *Calculate / Make Database*. Simple arithmetic operations and more complex trigonometric operations, but also lag-operations are available. The latter allow the inclusion of lag-effects as required by the methods L2, L3 and L4.

It should be noticed that the adjustment step requires the calculation of both the estimated load and the mean load. Therefore for every formula which contains the actual flow another formula has to be created which contains the long-term monthly mean instead of the actual flow. The long-term monthly mean is available in the variable *Base mean*. As an example the formulas for method L1 shall be described: It is - according to designation of the flow in the data bank (Q or Qdaily) - " 1 / Q " or " 1 / Qdaily ". The corresponding reference formula for the long-term monthly mean is " 1 / base mean ". It should be stressed that improper use of the formulas may lead to meaningless results or bring the program to a halt with an error message. The latter happens e.g. if mathematical and statistical requirements are not fulfilled.

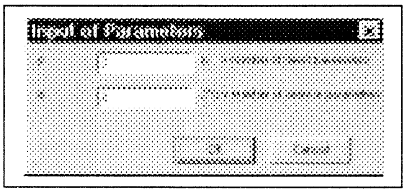
The formulas needed for adjustment have to be entered into the columns *Formulas Load estimated* and *Formulas load mean*. For several methods the formulas are available in the database and have simply to be activated. For example for the method L1 the formulas L1 and L1ref are to be activated in the columns *Formulas Load estimated* and *Formulas Load mean*, respectively. For the other adjustment method the formulas can be entered in an analogous way. This holds not only for the *Local regression* page, but also for the other pages *Stalnacke mod.*, *Hebbel* and *Spline*. Apart from the *Spline* page one may enter more than one formulas.

Finally the dataset has to be selected. This concerns the temporary tables which were created in the menu *Make database*. Open the drop-down list box on the toolbar and select one of the files. The station and the time period for the selection is displayed on the toolbar.

Press the button *Calculate* to calculate the formulas and to enter the results in the table *Time resolution*. This table can be displayed on the page *Result tables/charts*. However it is not absolutely necessary to activate the button *Calculate*.

In the next step the type of adjustment, the dependent variable (type of transformation) and the width of the window have to be fixed. If the calculations should be executed locally on the basis of a running window, enter the respective number of periods (85 months or 183 biweekly periods in case of a seven years window) into the field *Interval length*.

Finally the adjustment calculation has to be started by clicking the button *Start adjustment*. Thereupon a window opens in which the number of trend and seasonal parameters must be fixed. For the methods L1, L2 and L4 enter for both variables p=2 and q=2. Click the command button *OK* to continue the calculation process.

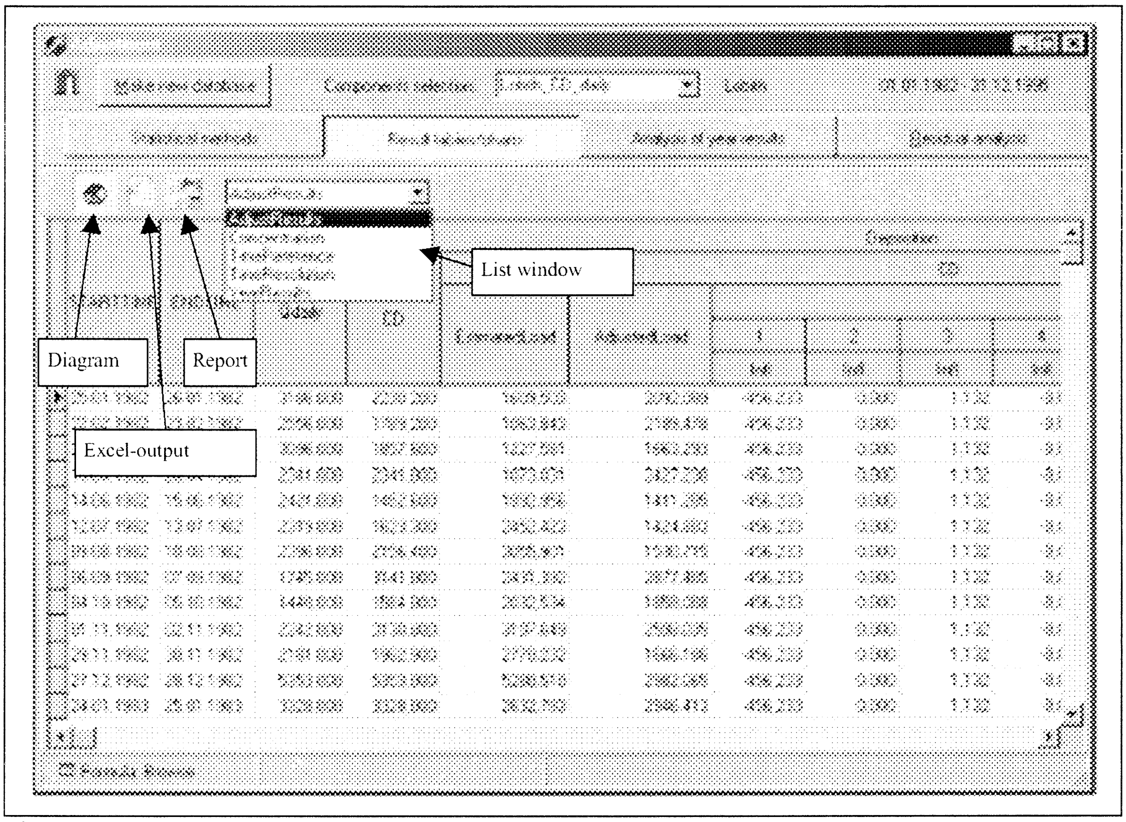


For the method L3 (without season modelling) enter p=2 and q=0.

In case of missing values or improper definition of formulas or improper setting of control parameters the calculation may stop if mathematical and statistical requirements are not fulfilled. In case of missing values it is recommended to activate the *Compress* option. This removes all data rows with missing values.

Screen shots for the different adjustment methods are represented in appendix 3.

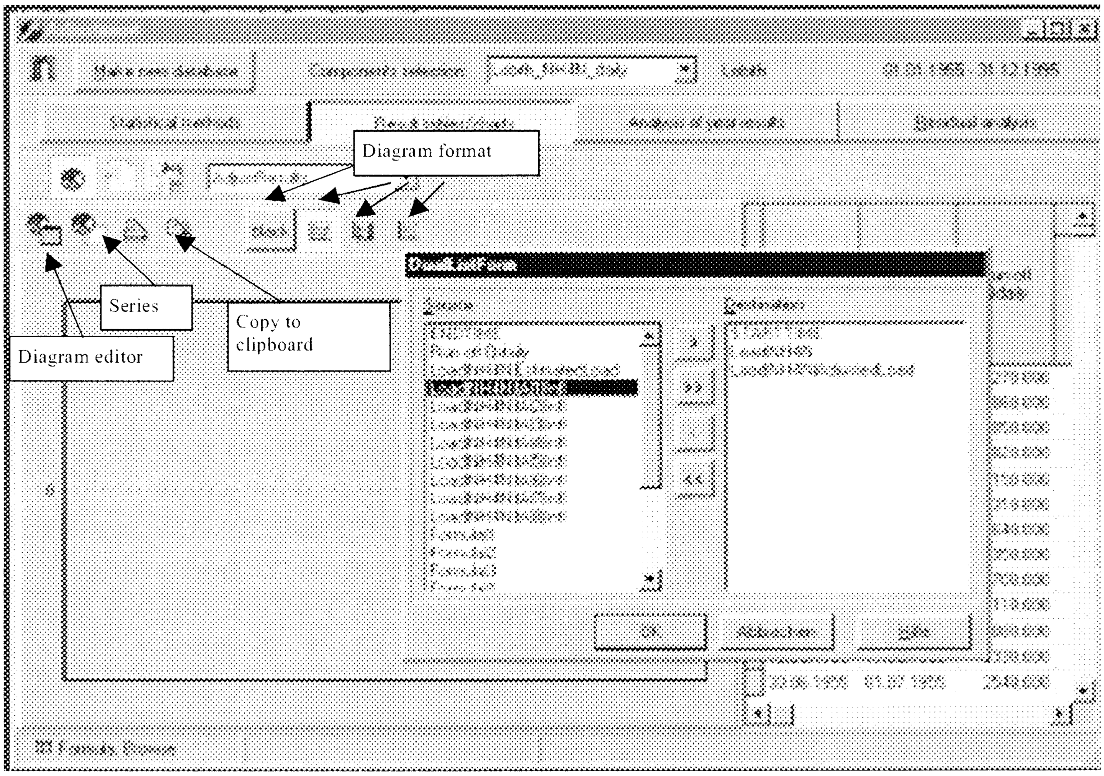
The results of the adjustment step and the subsequent aggregation step can be displayed in tables and diagram on the page *Result Tables/chart*. However, for the production of professional presentation graphics the diagram function is not suitable, particularly as it is not possible to display the results of several adjustment methods in one and the same diagram. The results of the Residual analysis can be made visible by clicking the command button *Residual analysis*.



Picture 24: Result tables

To open a specific table and to create a diagram or to prepare an EXCEL file, open the drop-down list box on the toolbar and select one of the files. With the command button *Report* the table can be transferred into a special report format. If the table does not fit on a sheet A4, an error message "table lines too long" is created. In this case the width of table columns should be manually reduced.

Simple diagrams of the tables can be created using the *diagram editor*. Click the button *Diagram* to activate the diagram. tool bar.

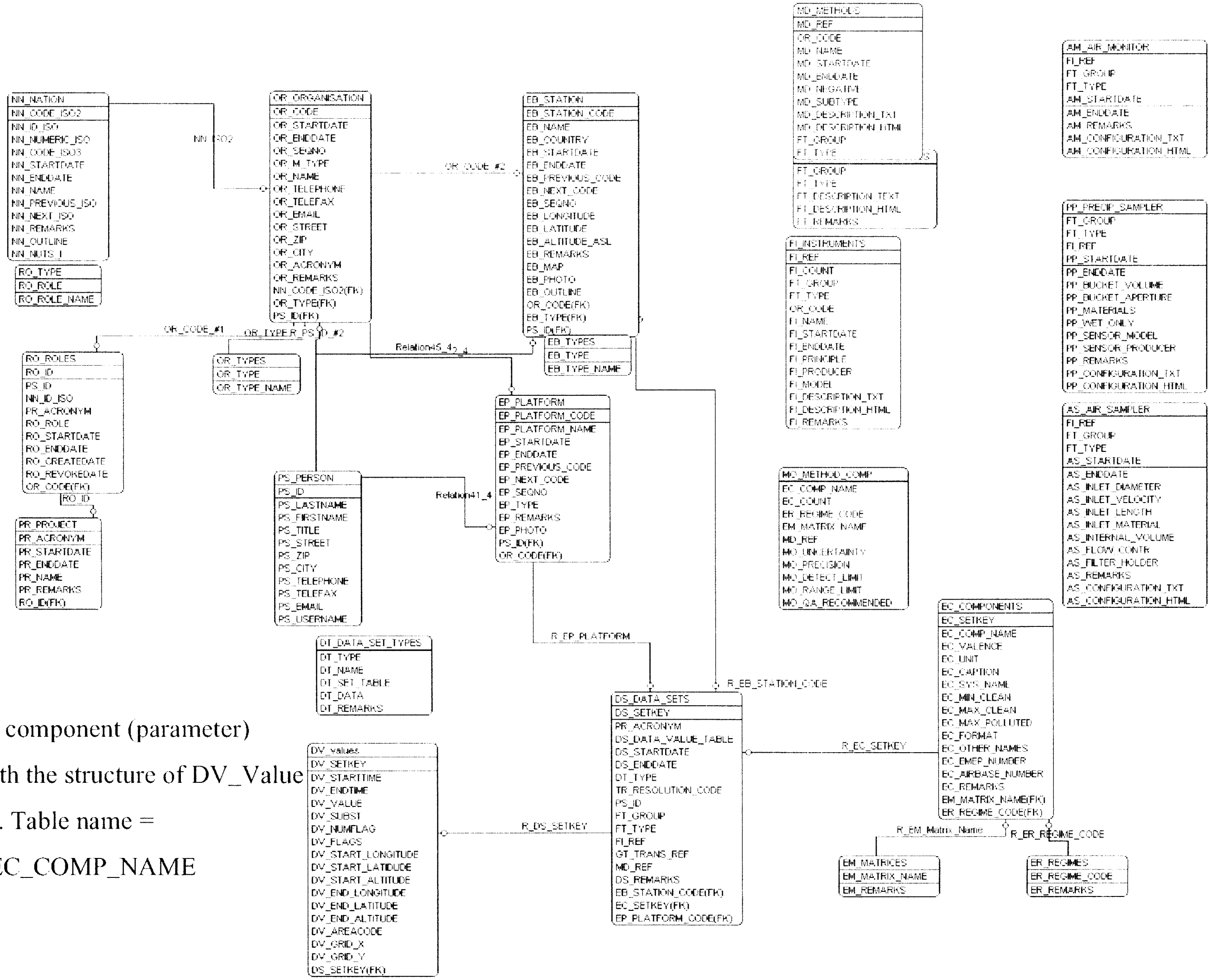


Picture 25: Selection of series for a diagram

By clicking on the command button *Series* a dialog window is opened for the selection of the series to be displayed. Highlight these series in the window *Source* and click the arrow pointing to the right. The columns are thereby transferred into the window *Destination*. The top row of this window contains the series which will be assigned to the "x-axis", while the remaining series are assigned to the "y-axis". If *START TIME* is the top series, the remaining series will be displayed as time series. Press the buttons referred to as *Diagram format* to select the diagram format (black-and-white, scatter diagram, line diagram, bar graph).

The final step of adjustment and trend analysis consists in calculating the smoother and the power function based on the annual adjusted loads. Click the command button *Analysis of year results* to obtain an EXCEL file with the trend analysis results.

Appendix 1 : Data base structure



For every component (parameter)

a table with the structure of DV_Value

is created. Table name =

DV_ + ' EC_COMP_NAME

Appendix 1: Data base structure

Appendix 2: Program structure of the program RTrend

The program is divided into following units:

About.pas
AdjustAndTablesRiv.pas
Adjustierung_FormularRiv.pas
Adressen.pas
CancelDialog.pas
ComponentCombinationRiver.pas
ConvertError.pas
DataBase_Tool.pas
Descript.pas
dmInstruments.pas
DM_Components.pas
DM_DataValue.pas
DM_MainTable.pas
EditComponents.pas
EditConverts.pas
EditDataset.pas
EditFormeln.pas
EditInstruments.pas
EditMainTables.pas
EditMeanValues.pas
EditOrganiType.pas
Einstellungen.pas
EvalFormula.pas
excel.pas
ExcelForm.pas
Exceltabs.pas
filter2.pas
Formelgenerator.pas
FUNKTIO.DLL
GeneralMessage.pas
Grid.pas
Histogramm1.pas
Import_Access.pas
Import_ExcelEintrag.pas
Import_ExcelMean.pas
Main.pas
MakeDB.pas
Makedb1.pas
MakeDS_Combination.pas
MakeInstrTypeDB.pas
nsUtils.pas
Progress.dfm
Progress.pas
QD_Matrizen.pas
QR2CONST.PAS
QRGridFormular.dfm
QRGridFormular.pas
Select4Stations.pas
SelectComponent1.pas
SelectMulti.pas
SelectStation.pas
SelectStation1.pas
SelectStationQR1.pas
SplineAdjustNeu.pas
StatusTableScan.PAS
TableOperation.pas
trend.inc
Trend01.vts
Trend02.vts
Trend03.vts
Trends_01_1.vts
VersionsInfo.pas

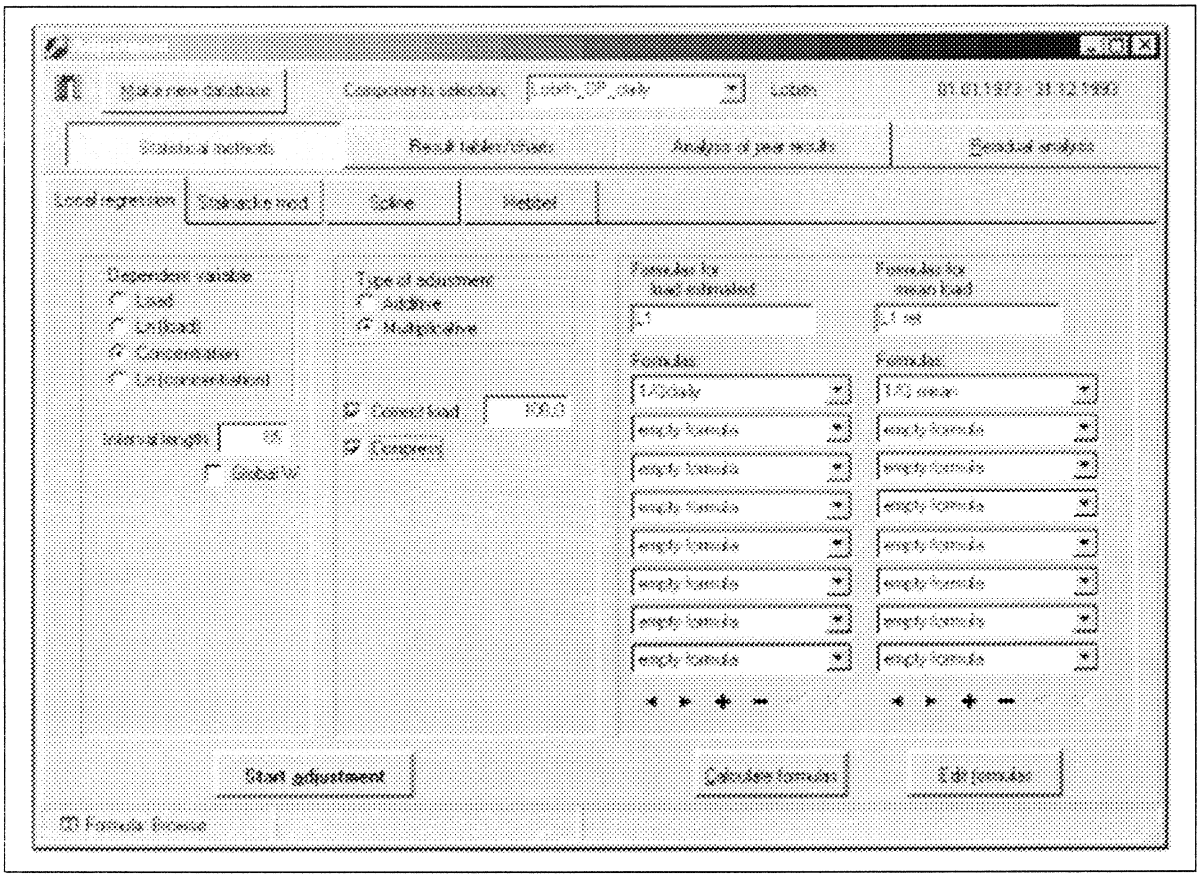
Appendix 3: Screenshots for the several adjusting methods

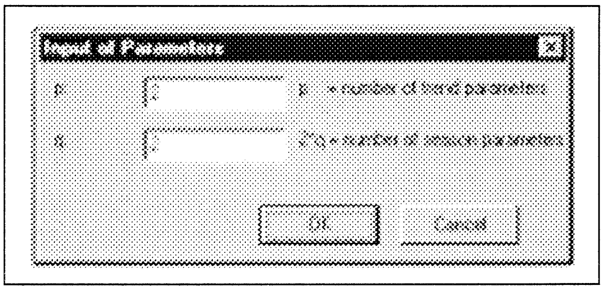
On the following pages the menu settings are represented for the different adjusting methods.

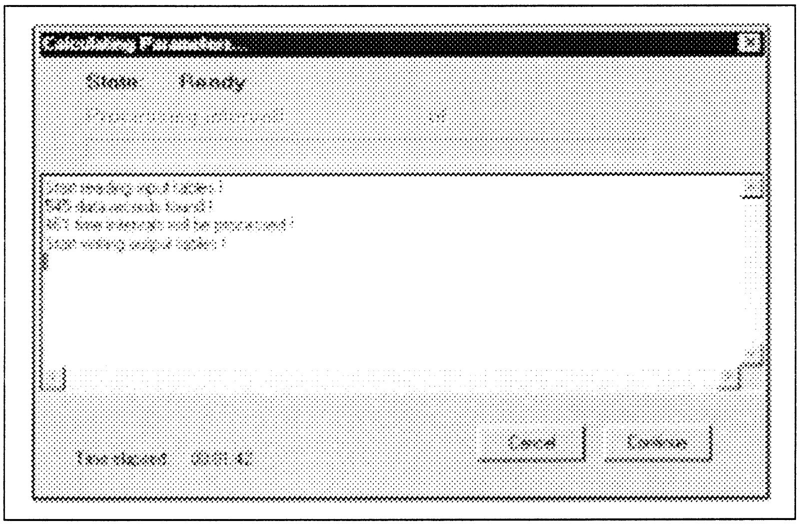
For all methods the definition of the interval length is to be paid attention to. The interval length depends on the temporal resolution of the data. If, for example, in accordance with method L1 a time window of 7 years is required, the interval length to be entered is 7x12 + 1 = 85 in case of monthly data, and 7x26 + 1 = 183 in case of biweekly data.

Furthermore, it should be noticed that all methods allow to enter a limit for the adjustment factor in accordance with section 5.11 (*correct load*). In the screenshots the limit 100 is entered, but other limits may be selected as well.

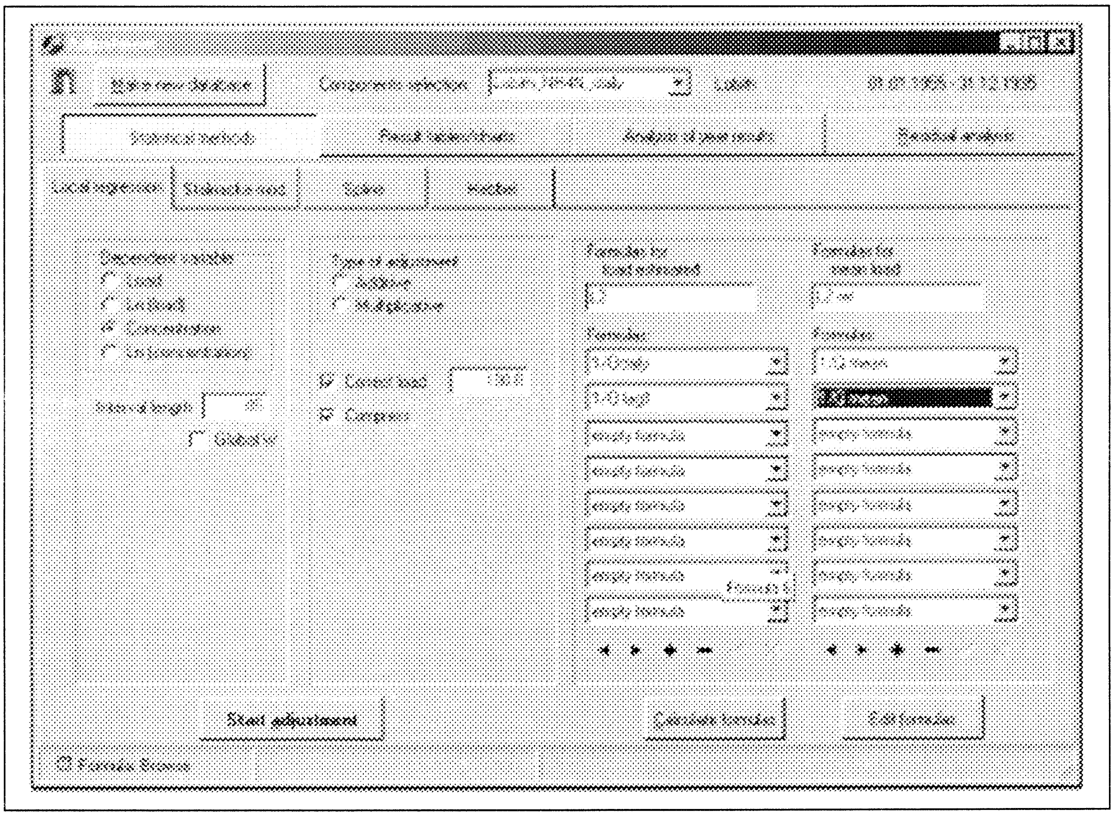
Linear regression with season (method L1)

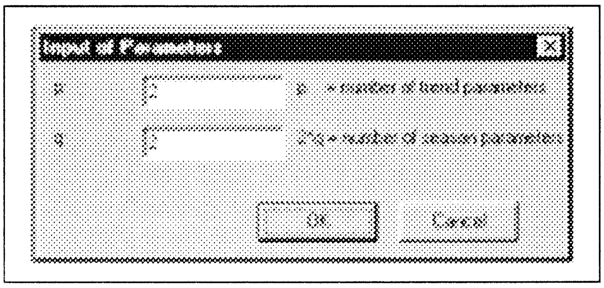


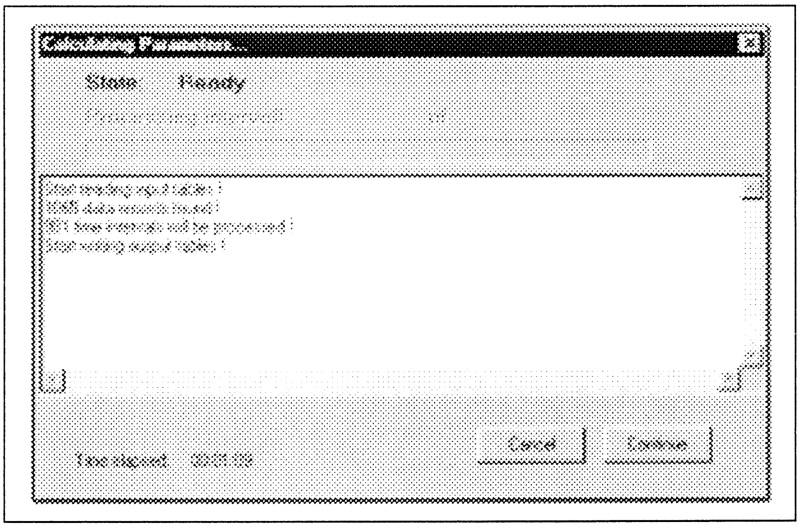




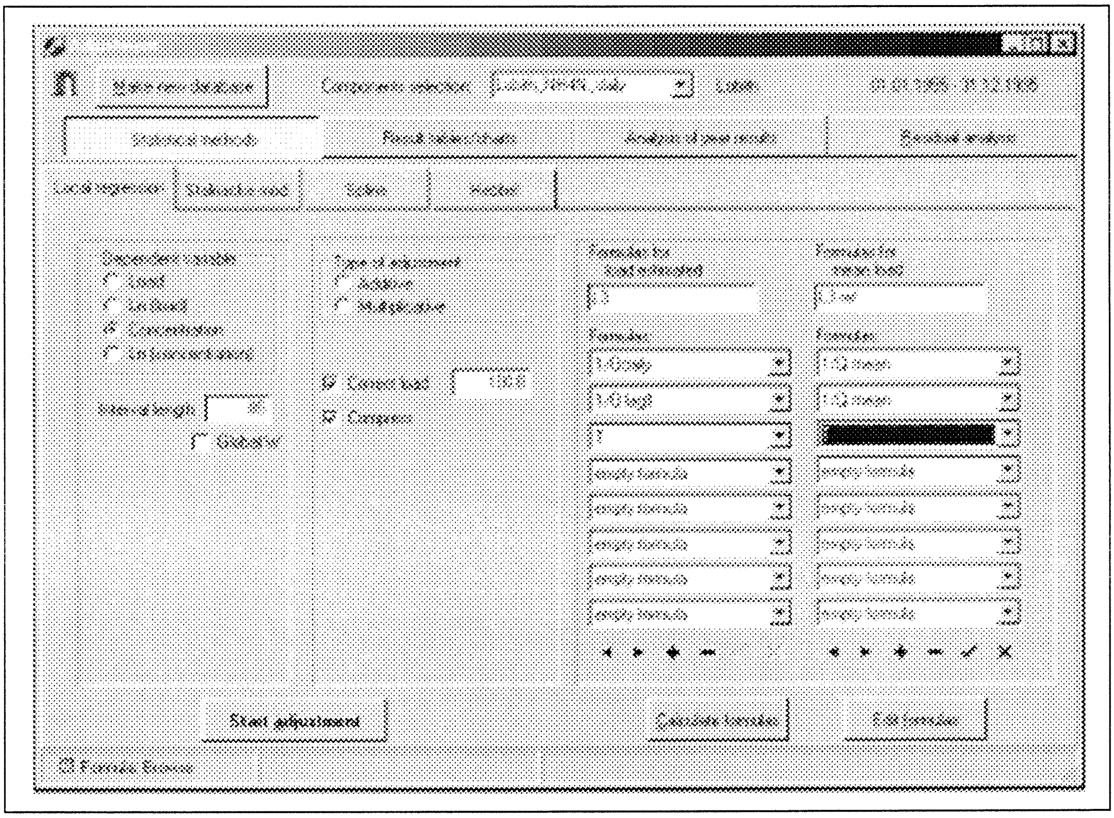
Linear regression with season and lagged runoff effect (method L2)

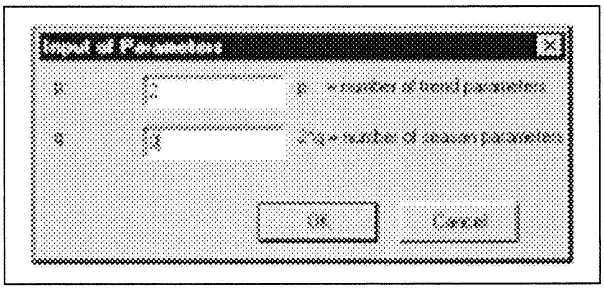


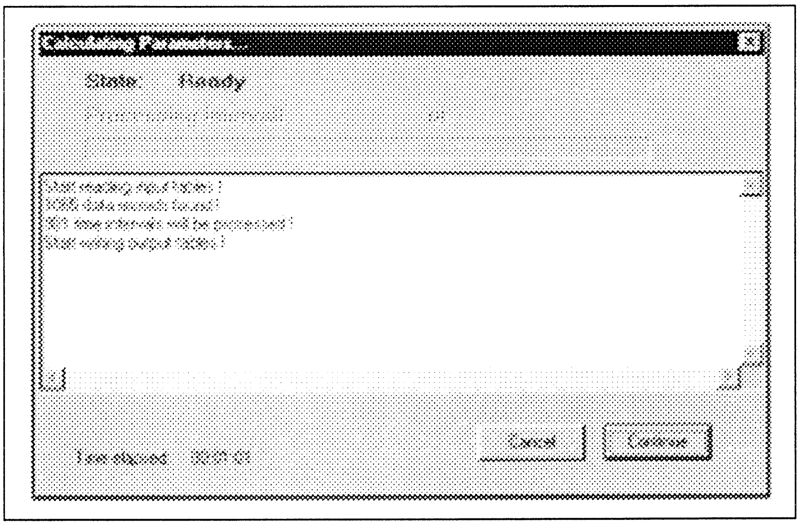




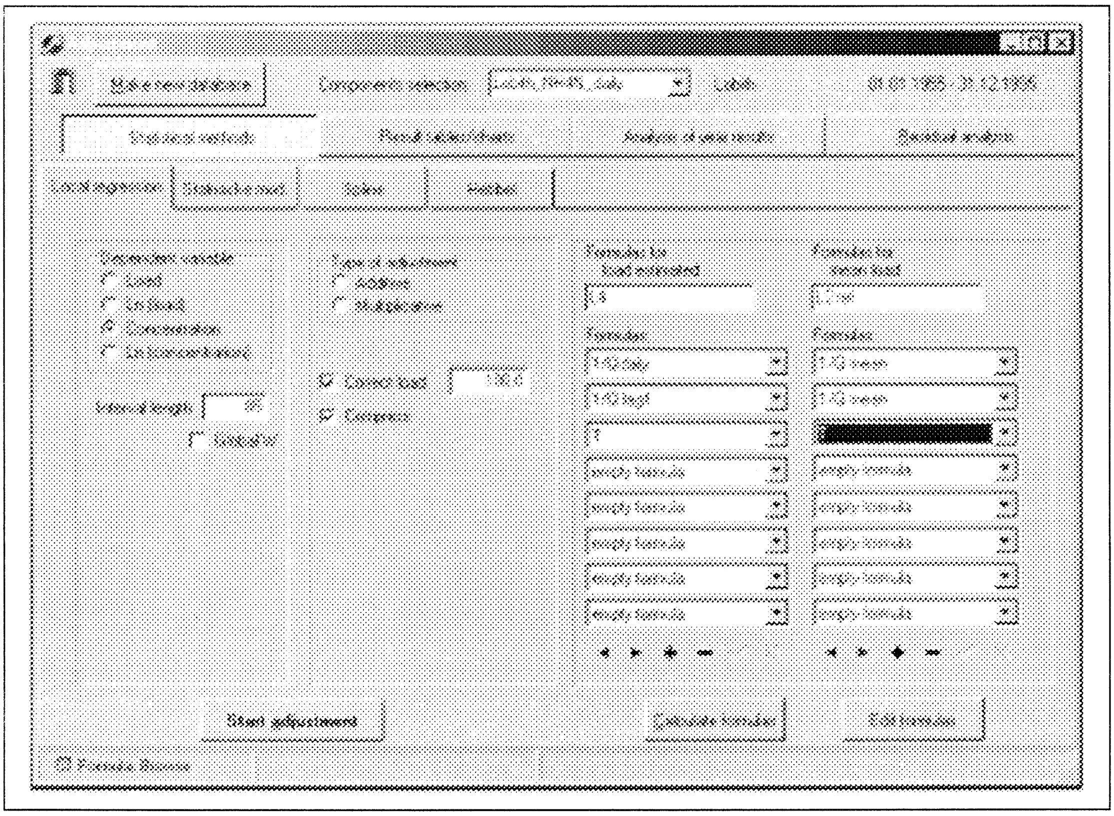
Linear regression with temperature and lagged runoff effect (method L3)

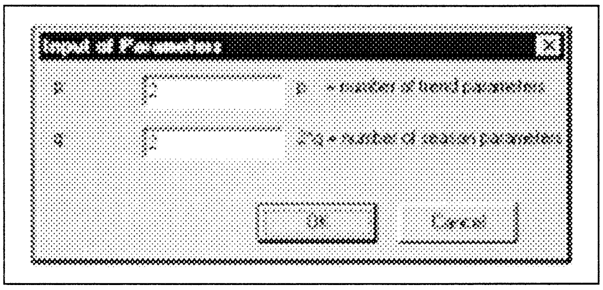


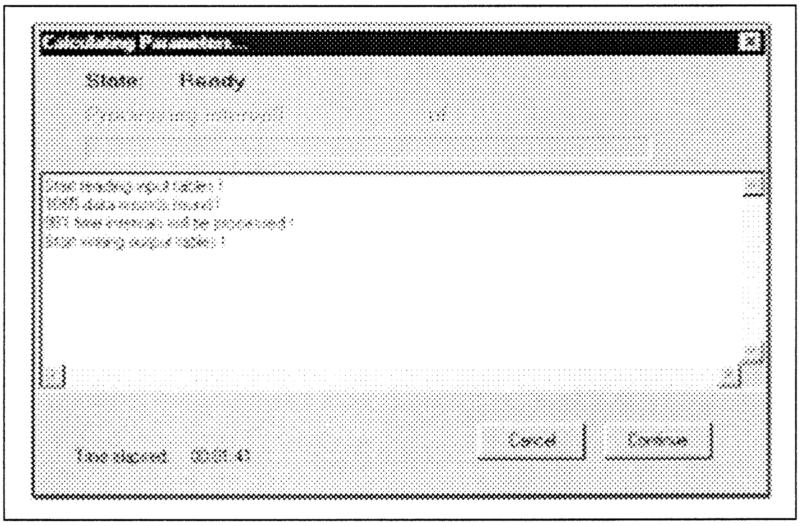




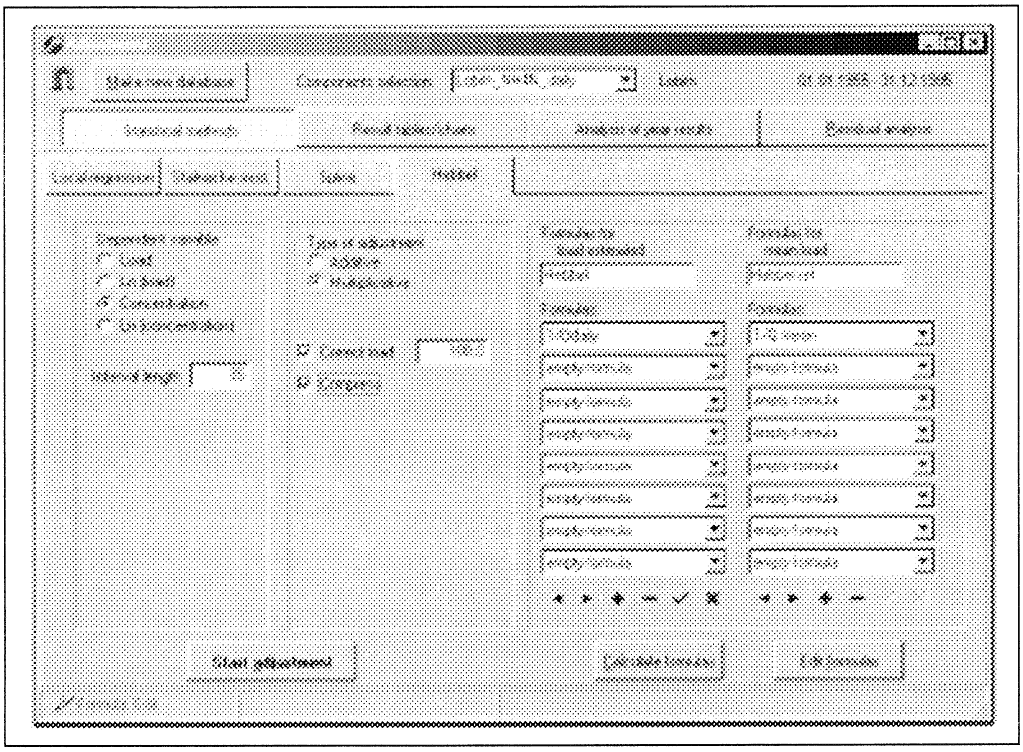
Linear regression with season, temperature and lagged runoff effect (method L4)

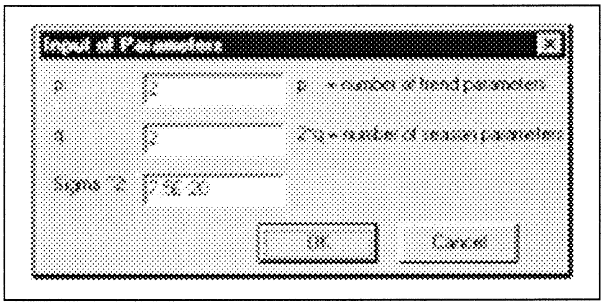


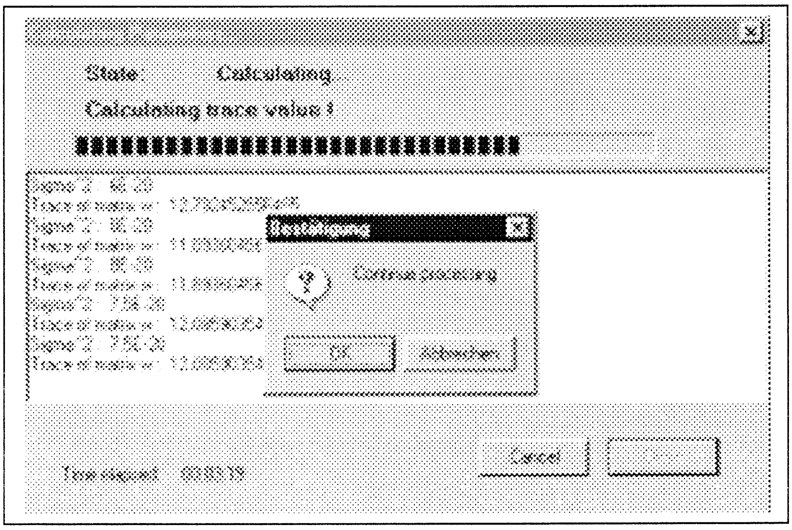




Application of the estimation procedure of Hebbel (method H)

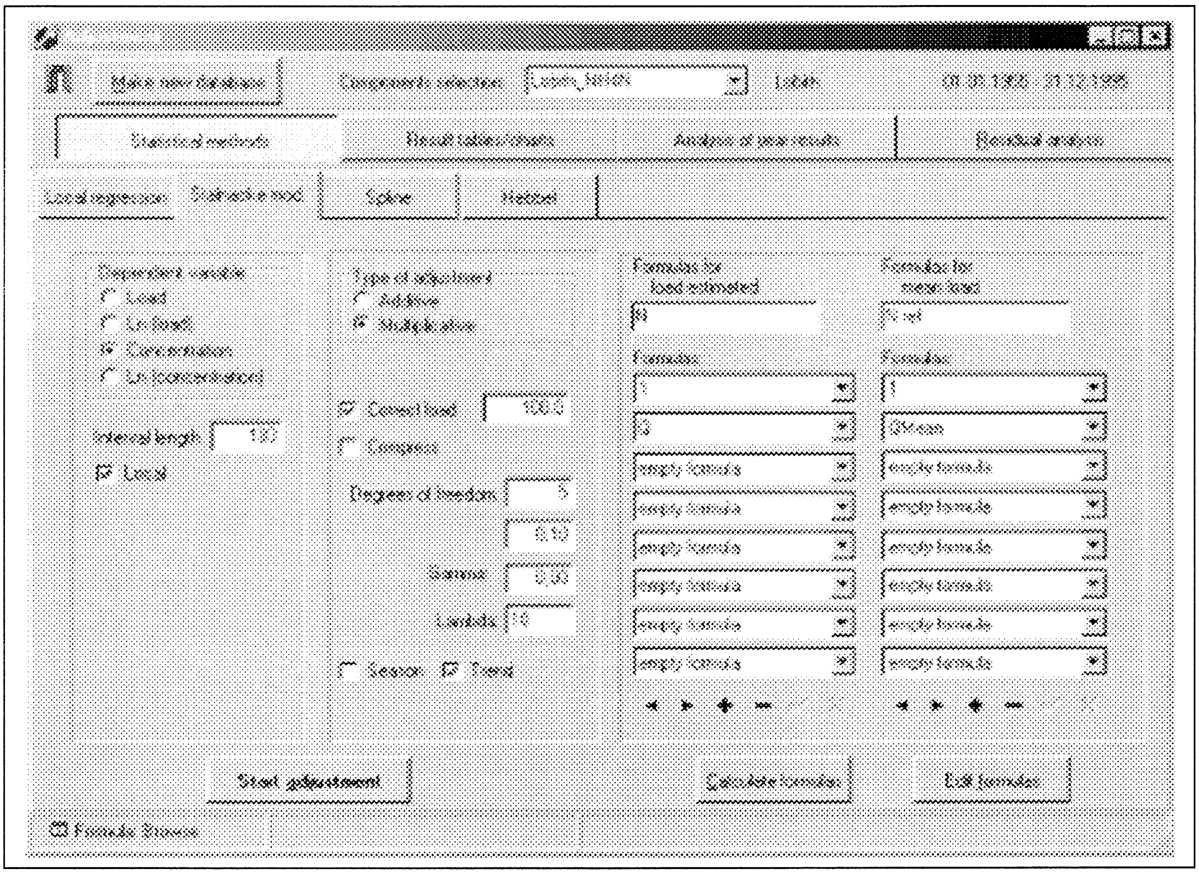


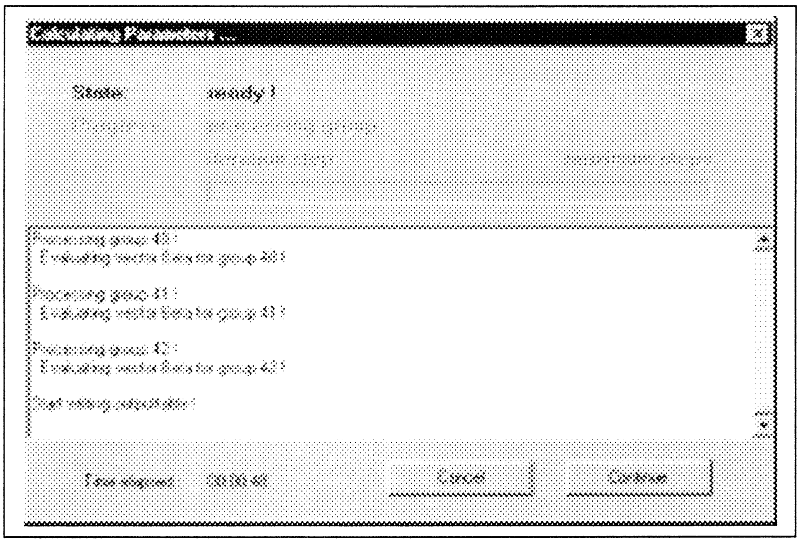




Sigma must be fixed so that the given number of 12 degrees of freedom (trace of matrix) is attained. As long as this criterion is not fulfilled yet, click the button named *Abbrechen* (in case of a German operating system) and select another value. The smaller Sigma is chosen, the larger is the number of the degrees of freedom.

Non parametric smoothing as per Stalnacke (method N):

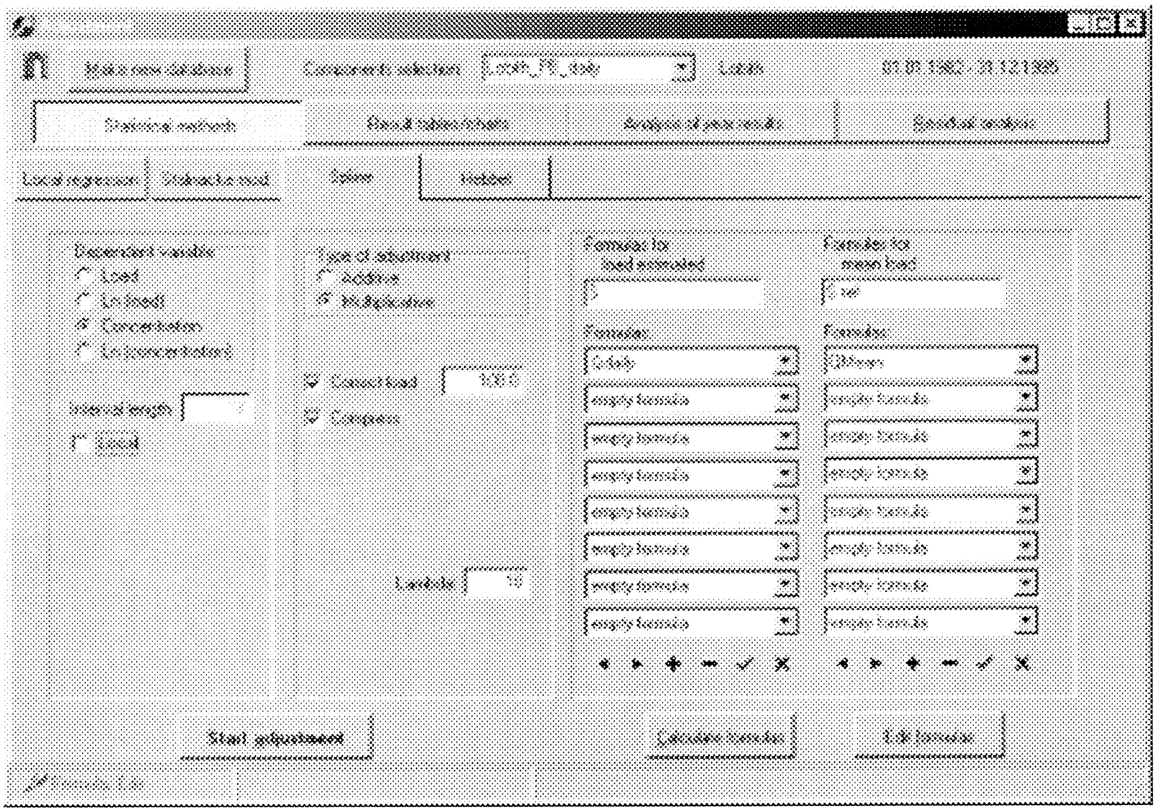




Method N requires monthly data. In the menu *Calculate / Make Database* for method N therefore the option *monthly* is to be applied instead of *daily*.

Estimation using Splines (method S1)

The parameter Lambda should be fixed (by trial) so that the trace of the smoother matrix equals four.



Estimation using local Splines (Method S2)

The parameter Lambda should be fixed (by systematic trying) so that the trace of the smoothing matrix equals four. The interval length of three years is expressed as number of successive periods. With biweekly measurements and 26 measurements per year the interval length of 78 has to be entered.