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Methodological aspects related to variations and uncertainties in empirical data needed to run and validate predictive models in coastal management – a general protocol

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EXECUTIVE SUMMARY

Even if measurement error could be completely eliminated, coastal ecosystems are inherently variable, and there are fundamental limits on the predictability of the temporal dynamics of many critical forcing functions. How do we incorporate the important sources of uncertainty in our ecosystem models and determine confidence in model output? How does uncertainty constrain our approaches to prediction? This work addresses these questions in discussing fundamental concepts in predictive ecosystem modelling, including optimal model size, predictive power, uncertainties in empirical y- and x-variables (y = target variable to be predicted; x = model variable), uncertainties in model structures, sensitivity analyses, uncertainty analyses (using Monte Carlo techniques) and uncertainties related to step-by-step predictions. Examples are given for aquatic ecosystems using both statistical regression models and dynamical mass-balance models based on differential equations. To meet demands in ecosystem management for generality, practical usefulness, and predictive power, models should not just be as small as possible and driven by readily accessible variables.

1. INTRODUCTION AND AIM

The variability and representativity of all model variables is a major concern in predictive modelling. Model variables may vary both within and among systems and the magnitude of these variations influences the predictive power of empirical models. For example, a given bioindicator may vary much in a coastal area during a month. Under calm conditions, it may be rather uniformly distributed in the water or it may change with water depth. During windy conditions, most bioindicators are likely to vary much areally and vertically (see, e.g., James and Barko, 1993; Bloesch, 1995; Weyhenmeyer, 1996). This means that there will be large uncertainties in single measurements. The same argument is valid not just for bioindicators in coastal management but all water variables in all aquatic systems.

This contribution may be seen as a paper on CV. CV is the coefficient of variation defined by the ratio between the standard deviation (SD) and the mean value (MV), i.e., CV = SD/MV. Different substances have different characteristic CVs (see table 1 for a compilation). In order to minimize model uncertainty, model variables with low CVs should preferably be used (Håkanson, 1999). Hopefully, this paper will demonstrate why this is important for all variables in all types of ecosystems.

Variations and uncertainties in empirical data constrain our approaches to knowledge about ecosystems and our possibilities to make meaningful predictions. This methodological paper addresses this question in discussing important concepts in predictive modelling in general. The focus here is not on concentrations but rather on CVs.

The first part concerns the following question: How high is the highest possible predictive success for a given target variable y? It is evident that many factors are involved concerning sampling (such as the number of samples), analysis (the method and precision used in determining y), temporal and spatial variations, model structure (which model variables x_i are included), the reliability of the model variables and the statistical methods used to define predictive success, e.g., the r^2-value (= the coefficient of determination; calculated from a regression between modelled values and empirical data of y). The r^2-value will be used here as a standard criterion of predictive success since this is a widely used concept in aquatic modelling (Håkanson and Peters, 1995). If a model is validated, i.e., tested against an independent set of data, the achieved r^2-value will not just depend on the uncertainty in the empirical y-value (i.e., the uncertainty in the y-direction), but also on the structuring of the model (i.e., which processes and model variables are accounted for and the empirical uncertainty of the model variables; the uncertainty in the x-direction). This paper will discuss three r^2-values:

1. The highest reference r^2 (r_r^2),
2. the empirically based highest r^2 (r_e^2) and
3. the achieved r^2 when modelled y-values are compared to empirical y-values (r^2).

To exemplify these concepts, this section will use empirical SPM-data from Håkanson (2005) and other literature data.

CV-values are probably the most commonly expressed statistic in contexts of ecosystem modelling (see Whicker, 1997). It is not likely that other statistical measures of uncertainty (see Gilbert, 1987) will substantially change the general conclusions about empirical uncertainties for aquatic variables discussed in this chapter.

2. BASIC CONCEPTS IN PREDICTIVE MODELLING

2.1. Modelling scale

A central problem in communications among scientists, and a key reason for much misunderstanding, has to do with scale. To model in great detail at the scale dealing with hourly or daily changes for target variables in water management is a very difficult task indeed for one system, and do this in a general, predictive manner for many systems is even more difficult. This is illustrated in fig. 1. This figure gives some important general concepts related to the "philosophy" behind the concept of scale in aquatic studies. The curve marked CV in fig. 1 illustrates how the uncertainty in empirical data increases if the data are collected during a day (a relatively small CV of 0.3), during weekly sampling within a system (a higher CV, 0.35), monthly sampling (a still higher value, CV = 0.55) and for samples collected over a year (CV = 0.95). The curve called "accessibility" illustrates that the overall sampling effort would increase, and the money and work related to the accessibility of data needed to run and test a model would also increase, for models based on daily predictions (e.g., using series of measured climatological data) to models for long-term predictions based on fewer and more readily available data from standard maps and/or monitoring programs. The bolded curve is meant to illustrate one of many possible ways to define the optimal size of a predictive model accounting for these two factors, the uncertainty in the empirical data (as given by CV) and the accessibility of the data (as given by N; where N is simply the number of days used for sampling; note that it is not meaningful to determine a mean value or a standard deviation from a sampling with fewer than three samples). Any model developer or user would have a set of criteria to define the practical usefulness of the model; different users may have different criteria. Given the bolded curve for practical usefulness in this figure, one can note that models striving for short-term (hourly - daily) predictions may not be very useful due to too high demands related to data accessibility, and that models based on annual predictions would generally be sub-optimal due to the high uncertainties in the empirical data. This motivates the scale in focus of the ecosystem models (mass-balance models for nutrients, SPM and toxic substances and a foodweb model) the Uppsala group aim to develop and test within the framework of the Thresholds project).

2.2. Highest r^2 of predictive models

Fig. 2 illustrates some fundamental concepts related to "the highest r^2". The data in the figure should emanate from several sampling occasions from a sampling site for defined time intervals (such as days, weeks or months). The CV-value for within site variability is always related to very complex climatological, biological, chemical and physical conditions. It has been shown (see table 1) that it is often possible to define a characteristic CV-value for a given variable, such as CV = 0.65 for SPM in lakes. Table 1 gives a compilation of such CV-values for many standard water variables from lakes, rivers, marine coastal areas and open water areas. By definition, CV is also largely independent of n, the number of data used to determine the mean value and the standard deviation, if n is large enough (n > 4). CV should also be independent of analytical method provided that the main difference between the methods can be expressed by a calculation constant ($y_1 = const \cdot y_2$). From table 1, one can note that:

• The characteristics inherent CV for individual SPM-data at river sites is very high indeed, 1.71. So, an important question is: How is it possible to reduce high CVs so that practically useful models may be derived, i.e., models giving r^2-values at least higher than 0.75?
• The highest reference r^2 (r_r^2) is lower than zero for SPM at many river sites. The achieved r^2-value can never be lower than zero but r_r^2 can. This will be explained in more detail in a coming section.
• The characteristic CV for SPM from individual marine open water sites is also very high, 0.67.
• The characteristic CV for SPM in lakes is 0.65, which is very high.
• The characteristic CV for SPM in marine coastal areas is 0.34, which is also a high value.
• Among all the studied water variables given in table 1, SPM has the highest inherent CV.

The uncertainty or variability associated with a given target variable is illustrated by the vertical uncertainty bands (error bars) in fig. 2. This uncertainty will evidently influence the result of regressions (e.g., the r^2-value when empirical and modelled data are compared). If CV for y is large, one cannot expect a model to predict y well. Fig. 2 illustrates a hypothetical model validation when modelled values of the target variable are put on the x-axis. The uncertainty in the x-direction is then related to the uncertainty associated with the model structure and the uncertainty of the model variables (x_i). Generally, one should expect the model uncertainty to be larger, or much larger, than the uncertainty in the y-direction. This is also illustrated in fig. 2.

The achieved r^2-value depends on the range of data. So, an important question is: How does the sample represent the population?

2.3. Empirically based highest r^2, r_e^2

One way to estimate the highest possible r^2 of a predictive model is to compare two empirical samples (r_e^2) since one can generally not expect models to predict better than empirical data. To illustrate this, SPM-data from River Avon (the station at Evesham; see Håkanson, 2005) will be used. Fig. 3 shows that the r^2-value calculated when comparing 32 samples taken within one week from two parallel series of data is 0.006 using actual data and 0.13 using logarithmic values. This includes analytical uncertainties but mainly depends on the very significant short-term (weekly) variability for SPM at this river site, which is also reflected in the very high characteristic CV of 1.71 for SPM in rivers. The higher the CV-value, the more difficult it will be to establish representative and reliable empirical mean values of the given variable. Evidently, r_e^2 depends on, e.g., the total number of samples in the regression and the number of samples for each individual value. The next r^2-value (r_r^2) has been defined as a standard reference r^2, which is meant to be independent of the sampling.

2.4. Highest reference r^2, r_r^2

An approach to estimate the highest reference r^2, r_r^2, has been presented and motivated by Håkanson (1999). This r^2-value only accounts for uncertainties related to the target y-variable (i.e., to CV for y). From a statistical point of view, an equation has been derived which gives the highest reference r^2-value as a function of (1) the number of samples (n_i) for each y_i-value in the regression, (2) the number of data points in the regression (N), (3) the standard deviations related to all individual data points, (4) the standard deviation of all points in the regression and (5) the range of the y-variable. The r_r^2-value is defined as:

$$r_r^2 = 1 - 0.66 \cdot CV_y^2 \qquad (1)$$

where CV_y is the characteristic within-site variability for the given y-variable. The equation is graphically shown in fig. 4. It is valid for actual (non-transformed) y-values. In practice in ecosystem modelling, one cannot expect to obtain r^2-values higher than the r_r^2-values, so these values may be used as reference values for practically useful predictive models.

Table 1 lists r_r^2-values for a number of water variables, some of these (e.g., salinity and pH) have low inherent CV-values and high r_r^2-values, and SPM is the opposite extreme.

2.5. The sampling formula and uncertainties in empirical data

If the within-site variability (CV_y or simply CV) is large, many samples must be taken to obtain a given level of certainty in the mean value. There is a general formula, derived from the basic definitions of the mean value, the standard deviation and the Student's t value, which expresses how many samples are required (n) in order to establish a mean value with a specified certainty (see Håkanson, 1999).

$$n = (1.96 \cdot CV/L)^2 + 1 \qquad (2)$$

where L is the level of error accepted in the mean value. For example, L = 0.1 implies 10% error so that the measured mean will be expected to lie within 10% of the true mean with the probability assumed in determining t. Since one often determines the mean value with 95% certainty (p = 0.05), the t-value is often 1.96 (or about 2).

The relationship between n, CV and L is illustrated in fig. 5. If the CV is 0.65 (the characteristic CV for SPM in lakes), then 163 samples are required to establish a site-specific mean value provided that one accepts an error of L = 10%. If one accepts a larger error, e.g., L = 20%, fewer samples are required. If, e.g., 4 samples are taken at a river site, the mean value may be estimated by an error of about 200%!

This illustrates that the variability/uncertainty of any water variable or bioindicator is fundamental in modelling, understanding and interpretations to causes to the variations(e.g, to thresholds) and hence also to remedial measures and strategies. An important question, which will be addressed below is: How would CV depend on the length of the sampling period? Evidently, individual data from specific sites and sampling occasions will represent the characteristic/mean/median conditions very poorly when the CV-value is high.

2.6. CV and sampling period

The data used in this example are measurements of SPM from River Avon (see Håkanson, 2005).

Fig. 6A exemplifies all actual (n = 93) data for SPM from this river site and fig. 6B gives the same data represented as monthly values with uncertainty bands (the box-and-whisker plots which give median values, M_{50}, quartile values, M_{25} and M_{75}, and percentiles, M_{10} and M_{90}). An important question concerns the characteristic CV-values based on daily, weekly, monthly and annual samples for the variable, since these CV-values regulate the predictive power (r_r^2; eq. 1) or the number of samples according to the sampling formula (eq. 2).

Table 2 shows 90 individual SPM data from this river site for the period 1994 to 1996. This table is included here to stress some important concepts. The column marked "MV, n = 6" shows mean values of the actual data for n = 6. One can note that the CV for n = 6 is 1.43, which is lower than the CV for the actual data, CV = 2.55. One should also note that the CV of 1.43 is significantly higher than the CV calculated when the actual data are randomly distributed in the given series, CV = 1.00. It is a standard practise in many statistical contexts to approximate the CV for a mean value according to eq. 3, but then one must also, as indicated in table 2, presuppose that the mean value comes from a random sample from a normal frequency distribution. The point here is that there are often seasonal or long-term trends in water variables and when this is the case, one cannot use this approach to reduce the CV without due reservations:

$$CV_{MV} \approx CV_{ind}/\sqrt{n} \qquad (3)$$

Where CV_{MV} is the CV for the mean and CV_{ind} is the CV for the individual data; n is the number of data used to determine the mean value.

Fig. 7A gives a compilation of CV-values calculated for mean values from weekly, monthly and yearly values, as well as the CV-value for all 459 individual data for chlorophyll-a in River Danube (Regensburg station; see Håkanson et al., 2003). The latter CV-value is 0.96 and in fig. 7A this value is compared to 19 similar values for chlorophyll for 19 sites in UK rivers (see Håkanson, 2005).

From fig. 7A, one can note:

• The mean CV for chlorophyll based on all data from the site in River Danube is close to the median value from 19 rivers sites in the UK.
• The daily, weekly, monthly and yearly CVs increase in steps from 0.3, 0.35, 0.55 to 0.95, respectively for chlorophyll.
• Analogous results have been obtained also for green algae, diatoms, cryptophytes and blue-greens (see Håkanson et al., 2003), and basically for all water variables, which is indicated in fig. 7B using data for SPM from River Avon.

3. MODEL TESTING

Calibration means that a given model set-up is tuned against empirical data so that the fit between modelled values and empirical data becomes as good as possible. All model variables in dynamic models (such as rates and distribution coefficients) could and should be tested, and there are generally several combinations of values for the model variables that can give good predictions when calibrated against a set of empirical data from one system. All such combinations cannot be correct if one seeks the model constants which could be used as general default values in model simulations for many systems. This means that calibrations often involve many iterations. The idea with the calibration procedure is that for each round of iterations the uncertainty in the values for the model variables should be reduced. When the model is properly calibrated, it should be validated, i.e., blind-tested against independent data. It is evident that it is preferable if the calibrations and the validations include as reliable empirical data from as many systems as possible covering as wide a range as possible in model variable characteristics.

3.1. Sensitivity tests

Sensitivity analysis involves the study of how an alteration of one model variable influences a given prediction, while everything else is kept constant. This analysis plays an important role in ecosystem modelling (see Hinton, 1993; Hamby, 1995; IAEA, 1998). This section gives an example of how a sensitivity analysis can be performed and the following chapter will give even more examples of this.

Fig. 8 gives a sensitivity analysis where the sedimentation of SPM, as calculated by the dynamic coastal SPM-model (see Håkanson et al., 2004), has been changed 100 times while all else in the model have been kept constant. The CV-value has been set to 0.5 for sedimentation from surface water to ET-areas (erosion and transport areas dominated by resuspension processes). From a normal frequency distribution with a mean value of 1 and a standard deviation of 0.5, 100 data have been drawn at random and used in the sensitivity test to produce the 100 curves for the target variable, modelled sedimentation on accumulation areas. It is evident from fig. 8, that the predictions of the y-variable is sensitive to how sedimentation on ET-areas (and hence also resuspension which depends on the amount of matter on ET-areas) is calculated. The uncertainty in y is also shown by the box-and-whisker plot in fig. 8B. One can note that when steady-state conditions have been reached, the CV-value for y is 0.32 related to the uncertainty in the given x-variable (here sedimentation on ET-areas).

The next step in a sensitivity analysis is often to repeat this type of calculation for all interesting model variables to try to produce a ranking of the factors influencing the target variable. The basic idea is to identify the most sensitive part of the model, i.e., the part that is most decisive for the model prediction. An example of such a comprehensive sensitivity analysis is given in fig. 9, again using the dynamic SPM-model for coastal areas

Fig. 9 gives the results when a uniform uncertainty (a CV of 0.5 and a normal frequency distribution around each mean value) has been used for all the fluxes in the coastal SPM-model. The idea is to rank the importance of the various uncertainties for the predictions of sedimentation on A-areas in this coastal area (Matvik, Sweden). From these presuppositions, one can note that the three most important uncertainties for this coastal area concern the SPM-fluxes in to and out of the surface water compartment (F_{outSW}, F_{inSW}, F_{SWET} and F_{SWDW}). All other uncertainties in the fluxes are of less importance and the uncertainty in land uplift (F_{LU}) is of no significance since land uplift is zero in this region. It may be realistic to use a uniform uncertainty for fluxes, but not for the driving variables. In the next test, the aim is to see how characteristic uncertainties in the driving variables will influence the uncertainty in the y-variable.

3.2. Uncertainty tests using Monte Carlo techniques

Two main approaches to uncertainty analysis exist, analytical methods (Cox and Baybutt, 1981; Beck and Van Straten, 1983; Worley, 1987) and statistical methods, like Monte Carlo techniques (Tiwari and Hobbie, 1976; Rose et al., 1989). In this section, Monte Carlo simulations will be discussed.

Monte Carlo simulations is a technique to forecast the entire range of likely observations in a given situation; it can also give confidence limits to describe the likelihood of a given event. Uncertainty analysis (which is a term for this procedure) is the same as conducting sensitivity analysis for all given model variables at the same time. A typical uncertainty analysis is carried out in two steps. First, all the model variables are included with defined uncertainties and the resulting uncertainty for the target variable calculated. Then, the model variables are omitted from the analysis one at the time. The procedure is illustrated in fig. 10.

Uncertainty tests using Monte Carlo techniques may be done in several ways, using uniform CV-values, or more realistically, using characteristic CV-values (e.g., from table 1). For practically useful predictive models based on several uncertain model variables (rates, etc.), the uncertainty in the prediction of the target variable (y) depends on such uncertainties. The cumulative uncertainty from many uncertain x-variables may be calculated by Monte Carlo simulations.

There are major differences among model variables in inherent CV (see table 1). Morphometric parameters can often be determined very accurately (see Pilesjö et al., 1991), some model variables, like rates and distribution coefficients, can, on the other hand, not be empirically determined at all for real water systems, but have to be estimated from laboratory tests or theoretical derivations. This means that the values used for such model variables are often very uncertain. Table 3 gives a compilation of typical, characteristics CV-values for different types of variables used in aquatic modelling. Note that in rivers, one should expect the CV for a given variable to be a factor of 1.5 to 2 higher than in lakes and coastal areas. From table 3, one can see that model variables like rates and distribution coefficients generally can be given CV-values of 0.5. High CV-values also appear for many sedimentological variables. In the following uncertainty tests, the CV-values given in table 3 are used.

The tests have been done for the following variables:

1. The concentration of SPM in the surface water outside the coast calculated from empirical data on Secchi depth, Sec_{SeaSW}. This is, as the previous sensitivity analyses indicated, a very important variable. The characteristic CV for Sec_{SeaSW} is set to 0.25.
2. The concentration of SPM in the deep water outside the coast (Sec_{SeaDW}). This is also a rather uncertain value and the characteristic CV is also set to 0.25.
3. The value used for the ET-areas (ET). This is an important distribution coefficient in mass-balance modelling and the ET-value in these simulations is predicted by an empirical sub-model. Those predictions are occasionally very uncertain. The characteristic CV is set to 0.5.
4. The theoretical surface water retention time (T_{SW}). This value is important because it regulates the fluxes of SPM to and from the sea and/or adjacent coastal areas. T_{SW} is calculated from an empirical model that has given an r^2-value of 0.95 (see chapter 6), but occasionally, the predicted T_{SW}-value is uncertain and CV is set to 0.25.
5. The theoretical deep water retention time (T_{DW}). T_{DW} is also calculated from an empirical model, which gave an r^2-value of 0.79. CV is set to 0.35.
6. Land uplift (LU). It is evidently very difficult to set a reliable CV for the influence of land uplift. The CV for LU is likely very high and set to 0.5.
7. The chlorophyll-a concentration regulating primary production. The CV is set to 0.25 (Wallin et al., 1992)
8. Salinity (Sal). There are comparatively reliable data on the salinity and the CV is set to 0.15.
9. The feed conversion ratio (FCR) influencing the point source emissions of SPM from a fish cage farm in this coastal area. CV is set to 0.1.
10. Surface water temperature (SWT); SWT is predicted from a modified version of a well-tested model and the CV-value is set to 0.1.
11. Finally, the coastal area. This value can be determined quite well but there may be uncertainties related to where the boundary line defining the coastal area is drawn. This CV is set to 0.05.

The aim now is to produce a ranking of these uncertainties for the target variable, sedimentation of SPM on A-areas (F_{DWA}).

Also the following test uses data for coastal area Matvik, Sweden (see Håkanson, 2005). The results are given in fig. 11. Note that:
• The total calculated CV for F_{DWA} according to this testing procedure is 0.83. The empirical CV for sedimentation in sediment traps is 0.5 (Wallin et al., 1992). This means that the

assumptions concerning the CV-values for the model variables should be reasonable. The CVs for the model variables should be set according to the precautionary principles so that the calculated CV is not smaller than the empirical CV.

• The most important factor is the uncertainty associated with the value used for the ET-areas. If this uncertainty is omitted, CV for F_{DWA} decreases the most, from 0.83 to 0.36. This means that future model development should concentrate on getting more reliable data and/or sub-models for the ET-areas.

• The model is not so well balanced since the model predictions depend much on one single uncertainty. In a well-balanced model, no part of the model dominates the calculated uncertainty in the target variables.

4. THE PARTITIONING COEFFICIENT, K_D

In aquatic ecosystems, substances in the water column can be divided into two main parts, the dissolved phase and the particulate phase, relating to their fates and transport routes (pelagic versus benthic). The distribution (= partition = partitioning) coefficient of substances depends on the association to suspended particulate matter (SPM). Predictive mass-balance models, obviously, should consider this particle association since it is a key factor regulating flows of substances in aquatic ecosystems. Particulate bound substances are, by definition, subject to gravitational sedimentation. Hence, they are to a high degree retained within the system and affect benthic habitats.

One well-known and general approach to describe the affinity of substances to carrier particles is by means of the partition coefficient, K_d (l/mg). K_d is generally defined as the ratio of filter-retained to filter-passing concentrations, e.g., calculated as:

$$Kd = (C_{part}/SPM)/C_{diss} \qquad (4)$$

where SPM is in mg/l, C_{diss} is the dissolved (filter-passing) concentration (mg/l) and C_{part} is the particulate concentration (mg/l).

In environmental investigations, total concentrations of trace substances are often found to increase with increased SPM (Cuthbert and Kalff, 1993; Balogh et al., 1997; Hurley et al., 1998a). For streams and rivers (Balogh et al., 1997; Kronvang et al., 1997; Solo-Gabriele and Perkins, 1997; Hurley et al., 1998a) and sediment resuspension (Slotton and Reuter, 1995), this is most often due to a marked increase in the particulate concentration of the given substance, C_{part}. Contradictory to this, K_d is generally found to decrease with increasing SPM. For trace metals and hydrophobic organic pollutants, the relationship with decreasing K_d with increasing SPM is well-known (e.g., O'Connor and Connelly, 1980; Duursma and Bewers, 1986; Honeyman and Santschi, 1988; Benoit et al., 1994; Benoit and Rozan, 1999; Turner et al., 1999). It is sometimes called "the particle concentration effect" and several mechanistic explanations have been suggested, e.g., sorption to colloids, filtration artefacts, particle-particle interactions, kinetics, qualitative variations in surface chemistry, irreversible adsorption or incomplete desorption (see Benoit, 1995). Slopes between $\log(K_d)$ and log(SPM) for trace metals found in environmental studies are generally in the range –1.0 to –0.5 (see Honeyman and Santschi, 1988) and for hydrophobic organic pollutants in the range –1.5 to –0.42 (from the compilation by Turner et al., 1999).

According to Johansson et al. (2001) the particulate fraction (PF, dimensionless; PF = $C_{part}/(C_{part}+C_{diss})$ is a much better alternative to K_d in mass-balance models for aquatic systems. There are three reasons for this conclusion:

1. PF is the variable that is actually necessary in mass-balance models since it, directly and not indirectly as K_d, describes and distributes mass flows of substances, which after all, is the goal of mass-balance models. To achieve the same mass flow distribution, the K_d-value must be recalculated into a PF-value.
2. As stressed, the CV-values vary between different substances and influence the predictive power of models. Table 4 gives a compilation of mean values and CV-values for many substances and different chemical forms of the substances (Ag, Cd, Co, Cr, Cu, Mn, Ni, P, Pb, and Zn) in many freshwater and marine systems. Since SPM is included in the calculations of K_d (eq. 3.3), but not of PF, the variability in SPM influences the CV for K_d. This is a major reason why CV for K_d is significantly larger than CV for PF, see fig. 12 which gives frequency distributions of CV-values for $C_{part,}$ C_{diss}, SPM, PF and K_d using the data given in table 4. One can note that the CVs for K_d generally are much (2-3 times) higher than for PF. This means that in mass-balance models, PF is preferable to K_d to distinguish between the dissolved and the particulate phases due to lower within-system variability.
3. Due to the definition of K_d as a ratio, spurious correlations may contribute to observed correlations between K_d-values and environmental variables (e.g., Kenney, 1982; Jackson et al., 1990; Krambeck, 1995). This means that regression models to varying degrees may overestimate correlations with variables that are included or closely related to any of the variables included in the K_d-ratio and this will be discussed in the next section.

4.1. Spurious correlations

There are at least two important areas in aquatic sciences involving spurious correlations, one concerns SPM and the distribution of substances into dissolved and particulate phases in the water, the other concerns river transport of SPM. These two cases will be addressed in the following section.

Spurious correlations is a fundamental statistical problem in situations where the y-variable is a function of x. To illustrate this, a random parameter test has been conducted where 100 random numbers have been generated for several variables which have then been regressed pair-wise and as ratios in the same manner as is done for real data to calculate K_d. So, SPM_{rand} represents randomly generated data that will be used in the same manner as real data for SPM are used; random values corresponding to total concentrations ($C_{totrand}$) and particulate concentrations ($C_{partrand}$) have also been produced. From these randomly produced data, PF (here called PF_{rand}) and K_d (here called K_{drand}) are calculated. Fig. 13A illustrates the regression between $\log(PF_{rand})$ and $\log(SPM_{rand})$. One can note that the spread around the regression line is, as it should be, totally random ($r^2 = 0.018$). However, there is a statistically significant ($p < 0.0001$) relationship between $\log(PF_{rand})$ and $\log(C_{partrand})$; $r^2 = 0.50$ because by definition $PF_{rand} = C_{partrand}/C_{totrand}$. The same situation is evident for $\log(K_{drand})$, see fig. 13D - there is a significant ($p < 0.0001$) relationship between the randomly produced values $\log(K_{drand})$ and $\log(C_{partrand})$ because K_{drand} is by definition equal to $(C_{partrand}/SPM_{rand})/(C_{totrand}-C_{partrand})$. By pure chance in this random parameter test, there is also a strong correlation between $\log(C_{partrand})$ and $\log(C_{totrand})$, $r^2 = 0.35$ (fig. 13F).

From these random parameter tests, one can conclude that there are several statistical problems in predicting ratios like PF, and the x-variables in regression models for PF should preferable not include C_{part} and C_{tot}, which by definition are used in defining PF.

It is a common practice in physical geography and hydrology to correlate sediment transport (e.g., in g/s; i.e., Q·SPM) on the y-axis with water discharge (Q in m^3/s) on the x-axis. This is spurious and the following test will demonstrate why. First, a random number generator has been used to produce 1000 random data called Q_{rand} and 1000 random data called SPM_{rand}. The correlation between these data is shown in fig. 14C; the r^2-value is 0.001. If the sediment transport is given on the y-axis as $\log(Q_{rand} \cdot SPM_{rand})$ and $\log(Q_{rand})$ on the x-axis, which is a “standard” practice in many contexts (see Jansson, 1982), there is a highly significant correlation ($r^2 = 0.49$, $p < 0.0001$), but it is spurious and a mathematical consequence of regressing a product against a component in the product. If 10 classes like the one shown in fig. 14A are used (to illustrate results from 10 different measurement stations), the results are shown in fig. 14B. The r^2-value is 0.973, a “perfect” correlation, but entirely spurious.

5. CONCLUSIONS ON PREDICTIVE POWER AND MODELLING

The predictive power of dynamic ecosystem models is determined by the model structure and the equations and model constants used for the various transport processes. If there is an error in the quantification of an important flux in a model, this error has to be corrected for by making at least one more compensatory error in order to calculate the target y-variable well in a given system. Any model can be tuned so that it describes empirical data well in a given system. However, errors in models are often - if not always - revealed when models are blind tested against independent data from new systems. So, validations are fundamental in ecosystem modelling in disclosing deficiencies in models and hence also in the modeller's understanding of how natural systems work. There are at least four basic criteria by which dynamic ecosystem models can be critically evaluated:

1. By the predictive power revealed by validations.
2. By the relevance of the target y-variable in disclosing fundamental ecosystem structures, functional aspects of aquatic ecosystems and threshold values related to operationally applied guidelines in water management.
3. By the applicability and generality of the model, i.e., by the width of the model domain. and
4. By the accessibility of the driving variables needed to make simulations.

There are a few key words that may be used to characterize scientific approach to modelling and understanding:

• Comparative studies. If the scientific task is to gain better understanding about how aquatic systems work, there are few more rewarding avenues than comparative studies. But comparative studies are based on data collected at individual sites, so there is no contradiction in studies based on different scale perspectives. Comparative study between different coastal areas and between lakes, rivers and marine areas should be fundamental in Thresholds and that perspective is not so common. Our project may also help to minimize the demarcation lines between academic disciplines.

• Process-oriented mass-balances. Statistical/empirical models may in themselves reveal very little about processes. However, such models are excellent tools to rank x-variables influencing variations in target y-variables, and in this way they can provide invaluable information in building practical and operational process-oriented mass-balance models. In such models, statistical explanation may be transformed into mechanistic explanation. Then, the aim is not to account for "everything", but to try to find and quantify the most important transport processes and omit or simplify the smaller processes. This is far easier said than done. But it can be done with the help of statistical/empirical modelling approaches. To find the optimal temporal and spatial scales for such dynamic process-oriented models is an important task, and also to find the most relevant modelling structure. The dynamic models for nutrients and toxins in lakes, rivers and coastal areas which we (the Uppsala group) will use in the project are all based on the same basic structure. The criteria to define the compartments, such as surface water, deep water, areas of erosion and transport and accumulations areas, are general and from these basic building blocks, one can also define algorithms for the key processes, such as sedimentation, resuspension, mixing, mineralization, production, inflow and outflow of X.

• Ecosystem perspective. All models used by the Uppsala group relate to the ecosystem scale, i.e., they are basically intended for entire defined coastal areas and for time periods of one month. This is also a very important perspective in water management, e.g., in contexts of impact assessment, when remedial measures are discussed and when very basic questions are asked, e.g.: What is the status on this ecosystem? What can be done to improve the conditions? Few people would be interested in the content of a sampling bottle. Most of us are interested in what this content may actually represent. That is, we are interested in a larger entity, the ecosystem. But there is no contradiction between work at this larger ecosystem scales and sampling and work at smaller scales, since the mean values characterizing ecosystem conditions and the standard deviations characterizing the variability around such mean values of necessity must emanate from sampling at individual sites.

• Practical usefulness. "Everything should be as small as possible, but not smaller". This statement from Albert Einstein is also a key to obtain practical usefulness of models for aquatic ecosystems. A very important demand for all models developed within the thresholds-project is that they should be practically useful, which implies that the obligatory driving variables should be easily accessed. The models should also predict well. The models we intend to develop in Thresholds should be driven by readily accessible data from standard maps and monitoring programs, e.g., altitude, latitude, continentality, area, mean depth and max. depth.

• Predictive power. The ultimate model testing is not sensitivity or uncertainty tests, like those discussed in the previous text, but validations, i.e., blind tests against independent data. For dynamic models at the ecosystem scale, it is very important to critically evaluate the area- and time-compatibility of the data when modelled values are compared to empirical data. Generally, one would assume that a poor fit between modelled values and empirical data can be explained by deficiencies in the model. But empirical data are, in fact, also always uncertain. This means that it is important to control model predictions against uncertainty bands for the empirical data. The dynamic models for SPM, phosphorus and toxins in coastal areas which we have today have been critically tested and demonstrated to give good predictive power. However, this does not mean that they will predict equally well for all systems. These models are meant to account for defined processes and factors in a general way so that the defined target variables can be predicted. Evidently, there may be situations which are not normal, but abnormal. Then, this modelling can provide a reference value, which would express normal conditions so that the divergency from the normal can be quantified and maybe related to the factor causing the abnormal conditions.

• Pluralism. Aquatic systems are very complex. This means that in order for science to progress concerning such systems, it is important to allow and stimulate different approaches, different models and pluralism. The modelling approaches used by the Uppsala group, and the scales and structures of these models, only provide one of many important pieces to the puzzle of modelling and understanding aquatic ecosystems. The argument here is that it would benefit science if competing and complementary approaches can be supported - not suppressed.

6. REFERENCES

Balistrieri, L.S., Murray, J.W. and Paul, B., 1992. The biogeochemical cycling of trace metals in the water column of Lake Sammamish, Washington: Response to seasonally anoxic conditions. Limnol. Oceanogr., 37: 510-528.

Balogh, S.J., Meyer, ML. and Johnson, D.K., 1997. Mercury and suspended sediment loadings in the lower Minnesota River. Environ. Sci. Technol., 31: 198-202.

Beck, M.B. and Van Straten, G., 1983 (eds). Uncertainty, system identification and the prediction of water quality. Springer, Heidelberg, 387 p.

Benoit, G., 1995. Evidence of the particle concentration effect for lead and other metals in fresh waters based on ultraclean technique analyses. Geochim. Cosmochim. Acta, 59: 2677-2687.

Benoit, G., Oktay-Marshall, S.D., Cantu, A., II, Hood, E.M., Coleman, C.H., Corapcioglu, M.O. and Santschi, P.H., 1994. Partitioning of Cu, Pb, Ag, Zn, Fe, Al and Mn between filter-retained particles, colloids, and solution in six Texas estuaries. Mar. Chem., 45: 307-336.

Benoit, G. and Rozan, T.F., 1999. The influence of size distribution on the particle concentration effect and trace metal partitioning in rivers. Geochim. Cosmochim. Acta, 63: 113-127.

Bloesch J., 1995. Mechanisms, measurement and importance of sediment resuspension in lakes. Mar. Freshwater Res., 46:295-304.

Cox, D.C. and Baybutt, P., 1981. Methods for uncertainty analysis: a comparative survey. Risk Analysis, 1: 251-258.

Cuthbert, I.D. and Kalff, J., 1993. Empirical models for estimating the concentrations and exports of metals in rural rivers and streams. Wat. Air Soil Pollut., 71: 205-230.

Duursma, E.K. and Bewers, J.M., 1986. Application of Kds in marine geochemistry and environmental assessement. In: T.H. Sibely and C. Myttenae (Editors), Application of distribution coefficients to radiological assessement models, Elsevier Applied Science Publishing Ltd, Essex, U.K., pp. 139-165.

Gilbert, R.O., 1987. Statistical methods for environmental pollution monitoring. Van Nostrand Reinold Co., New York.

Håkanson, L., 1999. Water pollution - methods and criteria to rank, model and remediate chemical threats to aquatic ecosystems. Backhuys Publishers, Leiden, 299 p.

Håkanson, L., 2004. Suspended particulate matter in lakes, rivers and marine systems. - The Blackburn Press, New Jersey, 331 p.

Håkanson, L. and Eckhéll, J., 2005. Suspended particulate matter (SPM) in the Baltic – New empirical data and models. Ecol. Modelling, 189: 130-150.

Håkanson, L., Gyllenhammar, A. and Brolin, A., 2004. A dynamic model to predict sedimentation and suspended particulate matter in coastal areas. Ecol. Modelling, 175: 353-384.

Håkanson, L., Malmaeus, J.M., Bodemar, U. and Gerhardt, V., 2003. Coefficients of variation for chlorophyll, green algae, diatoms, cryptophytes and blue-greens in rivers as a basis for predictive modelling and aquatic management. Ecol. Modelling, 169: 179-196.

Håkanson, L. and Peters, R.H., 1995. Predictive limnology. Methods for predictive modelling. SPB Academic Publishing, Amsterdam, 464 p.

Hamby, D.M., 1995. A comparison of sensitivity analysis techniques. Health Physics, 68:195-204.

Hinton, T. G., 1993. Sensitivity analysis of ecosys-87: an emphasis on the ingestion pathway as a function of radionuclide and type of disposition. Health Physics, 66:513-531.

Honeyman, B.D. and Santschi, P.H., 1988. Metals in aquatic systems. Environ. Sci. Technol., 22:862-871.

Hurley, J.P, Cowell, S.E., Shafer, M.M. and Hughes, P.E., 1998. Partitioning and transport of total and methyl mercury in the lower Fox river, Wisconsin. Environ. Sci. Technol., 32: 1424-1432.

IAEA, 1998. International Atomic Energy Agency. Modelling of radiocesium in lakes. Tec. Doc. (in print), Vienna.

Jackson, D.A., Harvey, H.H. and Somers, K.M., 1990. Ratios in aquatic sciences: Statistical shortcomings with mean depth and the morpoedaphic index. Can. J. Fish. Aquat. Sci., 47:1788-1795.

James, W.F. and Barko, J.W., 1993. Sediment resuspension, redeposition, and focusing in a small dimictic reservoir. Can. J. Fish. Aquat. Sci., 50: 1023-1028.

Johansson, H., Lindström, M. and Håkanson, L., 2001. On the modelling of pariculate and dissolved distributions of substances in aquatic ecosystems – sedimentological and ecological interactions. Ecol. Modelling, 137:225-240.

Kenney, B.C., 1982. Beware of spurious self-correlations! Wat. Resour. Res., 18:1041-1048.

Krambeck, H.-J., 1995. Application and abuse of statistical methods in mathematical modelling in limnology. Ecol. Model., 78:7-15.

Kronvang, B., Laubel, A. and Grant, R., 1997. Suspended sediment and particulate phosphorus transport and delievery pathways in an arable catchment, Gelbæk stream, Denmark. Hydrol. Process., 11: 627-642.

Nordvarg, L., 2001. Predictive models and eutrophication effects of fish farms . Dr. Thesis, Uppsala University, Sweden.

O'Connor, D.J. and Connelly, J.P., 1980. The effect of concentration of adsorbing solids on the partition coefficient. Wat. Res., 14: 1517-1526.

Pohl, C. and Hennings, U., 1999. The effect of redox processes on the partitioning of Cd, Pb, Cu, and Mn between dissolved and particulate phases in the Baltic Sea. Mar. Chem., 65: 41-53.

Rose, K.A., McLean, R.I. and Summers, J.K., 1989. Development and Monte Carlo analysis of an oyster bioaccumulation model applied to biomonitoroing. Ecol. Mod., 45:111-132.

Slotton, D.G. and Reuter, J.E., 1995. Heavy metals in intact and resuspended sediments of a California reservoir, with emphasis on potential bioavailability of copper and zinc. Mar. Freshwat. Res., 46: 257-265.

Solo-Gabriele, H.M. and Perkins, F.E., 1997. Metal transport within a small urbanised watershed. J. Irrig. Drain. Enging., 123: 114-122.

Talbot, R.W. and Andren, A.W., 1984. Seasonal variations of ^{210}Pb, and ^{210}Po concentrations in an oligotrophic lake. Geochim. Cosmochim. Acta, 48: 2053-2063.

Tiwari, J.L. and Hobbie, J.E., 1976. Random differential equations as models of ecosystems. Monte Carlo simulation approach. Math. Biosci., 28:25-44.

Turner, A., Hyde, T.L. and Rawling, M.C., 1999. Transport and retention of hydrophobic organic micropollutants in estuaries: Implications of the particle concentration effect. Estuar. Coast. Shelf Sci., 49: 733-746.

Wallin, M., Håkanson, L. and Persson, J., 1992. Load models for nutrients in coastal areas, especially from fish farms (in Swedish with English summary). Nordiska ministerrådet, 1992:502, Copenhagen, 207 p.

Weyhenmeyer, G.A., 1996. The significance of lake resuspension in lakes. Uppsala dissertations from the faculty of science and technology 225. Sweden. ISBN 91-554-3820-2.

Whicker, F.W. and Schultz, V., 1982. Radioecology: Nuclear energy and the environment. Volume 1, CRC Press, Boca Raton, 228 p.

Worley, B.A., 1987. Deterministic uncertainty analysis. Oak Ridge National Laboratory Report ORNL-6428, Oak Ridge, U.S.A., 53 p.

Fig. 1. Illustration of factors regulating the optimal size of practically useful predictive models in water management. The curve marked N illustrates the accessibility (number of data); the CV-curve illustrates uncertainties in empirical data; and the bolded curve gives one expression for the optimal temporal scale related to the CV-curve and the N-curve (from Håkanson, 2005).

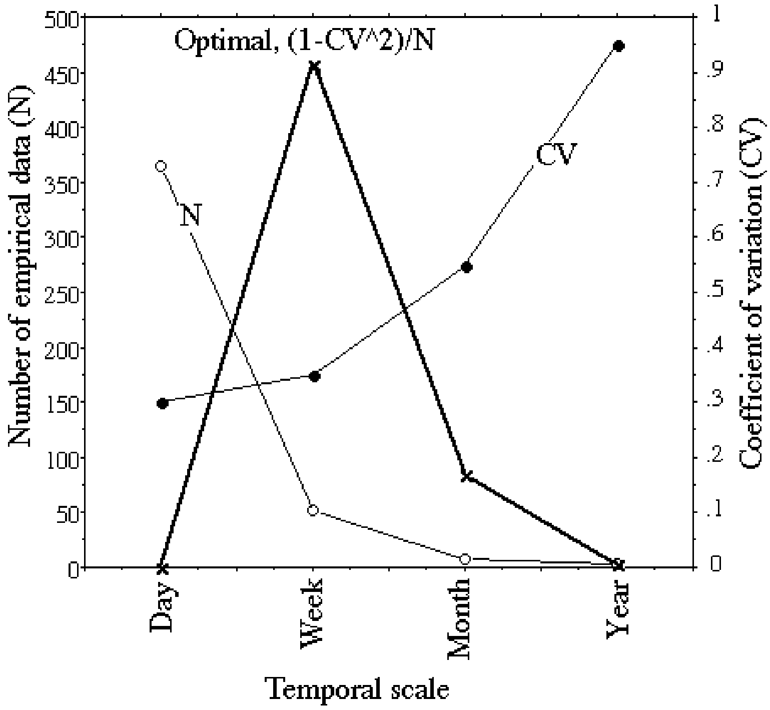

Fig. 2. Illustration of fundamental concepts related to the question of "the highest possible r^2" of models as determined from validations, i.e., a comparison between modelled values (on the x-axis) and independent empirical data on the y-axis. Note that the uncertainty in the y-direction (e.g., given by the CV-value) differs among variables and that the characteristic uncertainty in the y-direction regulates the predictive power of the model.

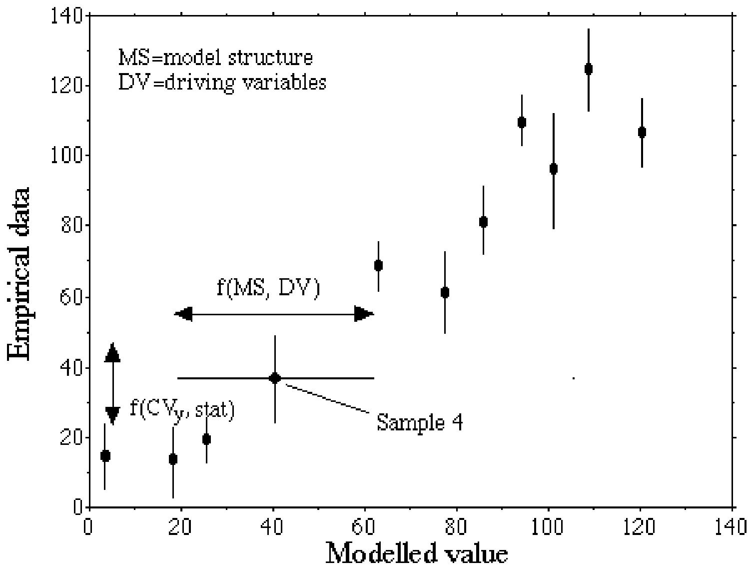

Fig. 3. Example illustrating determination of "empirically highest r^2" (r_e^2) for SPM from a regression between two parallel empirical samples taken within a week (Emp_1 vs Emp_2). The r_e^2-value is 0.006 for the given 32 data-pairs for SPM in the River Avon (data from appendix 9.1).

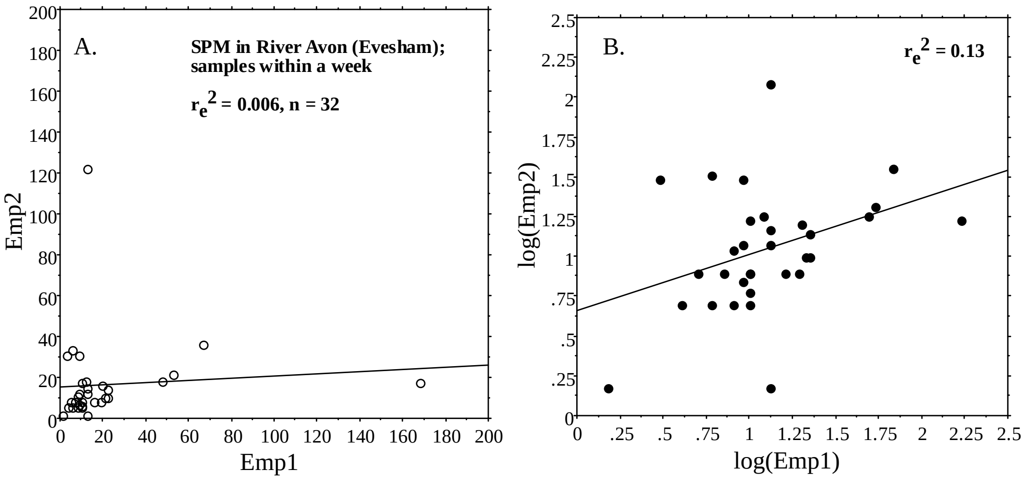

Fig. 4. The relationship between the "theoretically highest reference" r^2 (r_r^2) and the coefficient of variation for variability within (CV_y) ecosystems. Figure modified from Håkanson (1999).

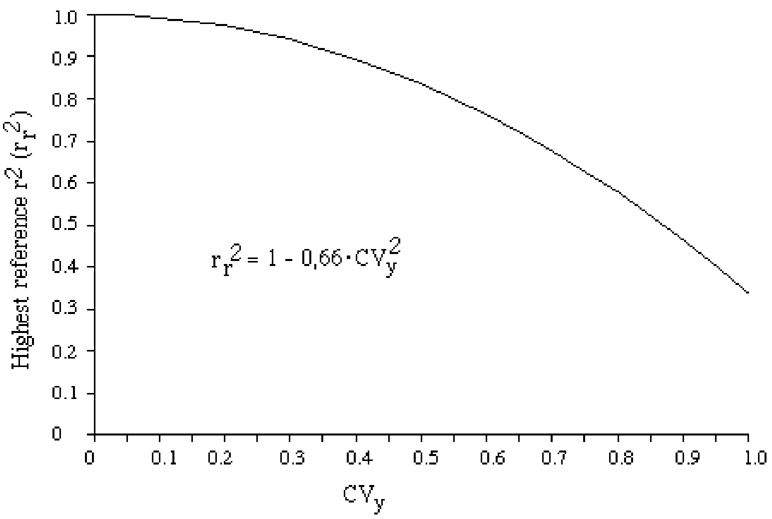

Fig. 5. Illustration of the sampling formula. The nomogram shows how many samples that must be analysed (n) to establish a characteristic mean value (MV) with a given uncertainty or error (L) and a given confidence (95%).

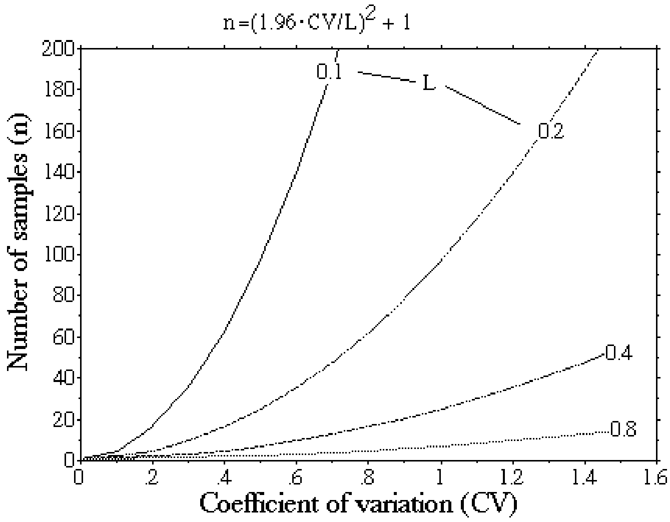

Fig. 6. A. All actual data (n = 92) from the sampling site in River Avon (Evesham station) for SPM 1994 to 1996.

B. The same data but calculated as monthly values and the corresponding uncertainty bands (medians, M_{50}, quartiles, M_{25} and M_{75}, percentiles, M_{10} ands M_{90} and outliers). From Håkanson (2005).

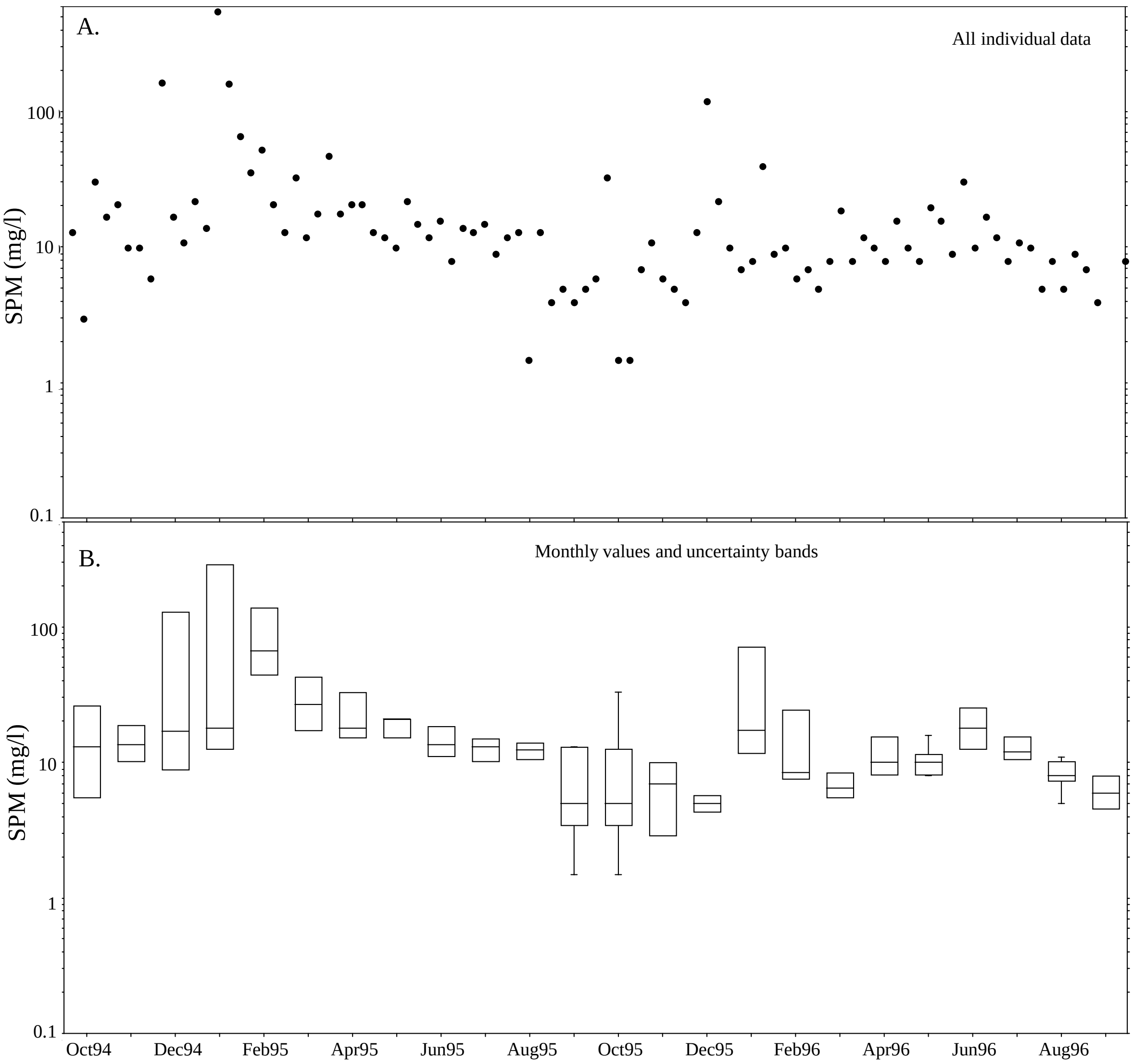

Fig. 7. Compilation of CV-values based on mean values from different time intervals, daily, weekly, monthly (from individual months and monthly data from several years), yearly and all data from 1995-1999 for chlorophyll from the River Danube (Regensburg station). The box-and-whisker plot to the right gives for comparative purposes CV-values based on all data from several years from 19 UK rivers. The results for the UK rivers sites should be compared to the CV-value of 0.96 calculated using all data from the Regensburg station (from Håkanson et al., 2003).
B. Gives corresponding information for SPM in River Avon, UK. From Håkanson (2005).

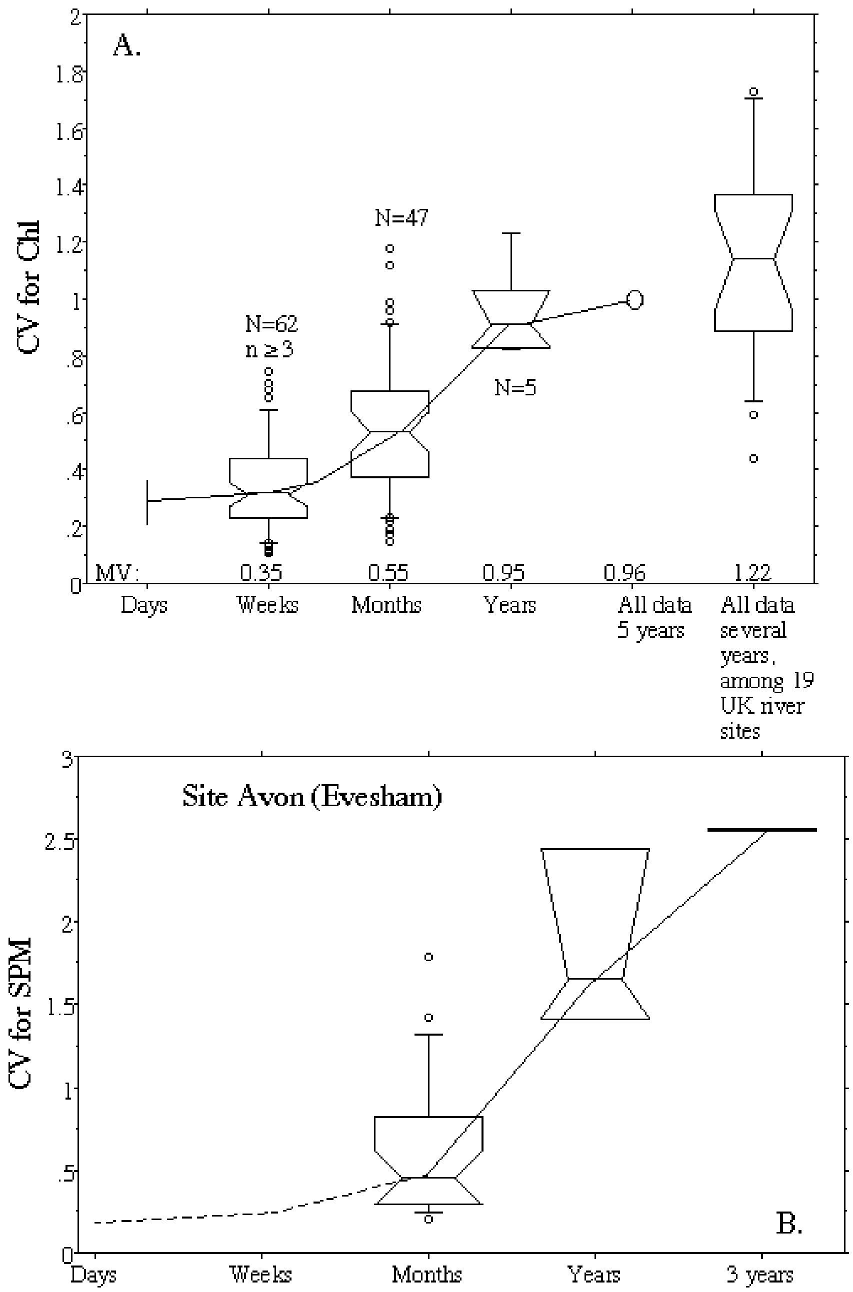

Fig. 8. A. Results from a sensitivity test (100 runs) using the dynamic coastal model for SPM (see chapter 6) and data for the coastal area Matvik, Sweden. The uncertainty for one of the fluxes, sedimentation from surface water to ET-areas, is defined by a CV of 0.5 and by a normal frequency distribution around the mean, and all else have been kept constant. The idea is to study how this uncertainty influences the uncertainty in the given target variable, sedimentation on accumulation areas. For the following tests, data from July (month 31) have been selected, as indicated in the figure.

B. Gives the corresponding box-and-whisker plot and statistics (CV for y = 0.32). Figure from Håkanson et al. (2004).

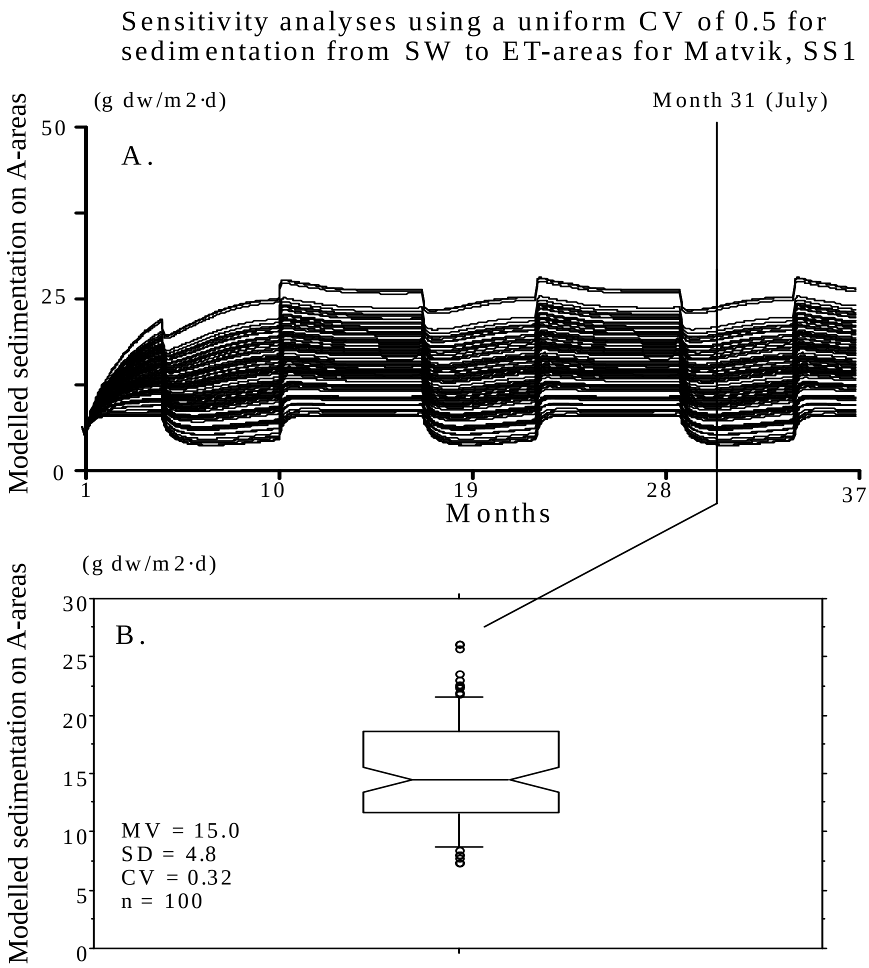

Fig. 9. Sensitivity tests where all fluxes in the coastal SPM-model are accounted for, one by one and all else kept constant. In this example, a uniform uncertainty has been used for all the fluxes (a CV of 0.5 and a normal frequency distribution around the mean value). The idea is to rank the importance of the fluxes in relation to the prediction of the target variable, sedimentation on A-areas, under these presuppositions for this coastal area (Matvik, Sweden). The figure gives the box-and-whisker plots (median, 25 and 75 quartiles, 10 and 90 percentiles and outliers) as well as the CV for the y-variable (e.g., 0.8 related to the uncertainty in the flux of SPM from surface water in July). From Håkanson et al. (2004).

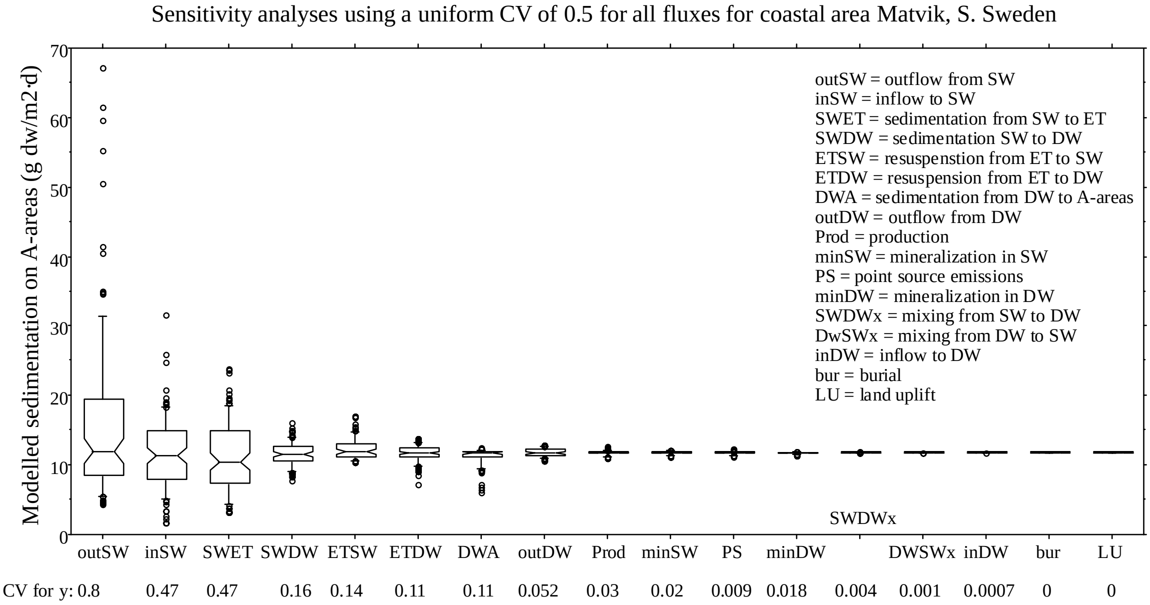

Fig. 10. Illustration of the principles of uncertainty analysis using Monte Carlo simulations.

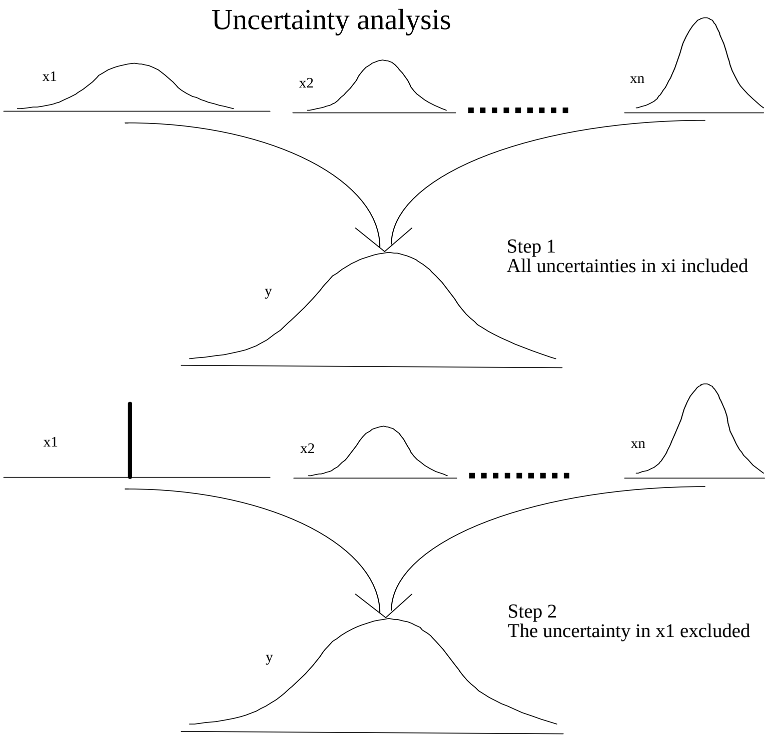

Fig. 11. Uncertainty analyses using Monte Carlo techniques using data for area Matvik, Sweden for the target variable, sedimentation on A-areas. The figure gives characteristic CVs for the eleven selected driving variables (e.g., 0.5 for ET, 0.15 for salinity and 0.05 for coastal area), calculated CVs for sedimentation (e.g., 0.83 when all these uncertainties are accounted for at the same time and 0.36 when the uncertainty for ET is neglected and all other uncertainties are accounted for) and a ranking based on the calculated CVs of how uncertainties in these driving variables influence the uncertainty for sedimentation. From Håkanson et al. (2004).

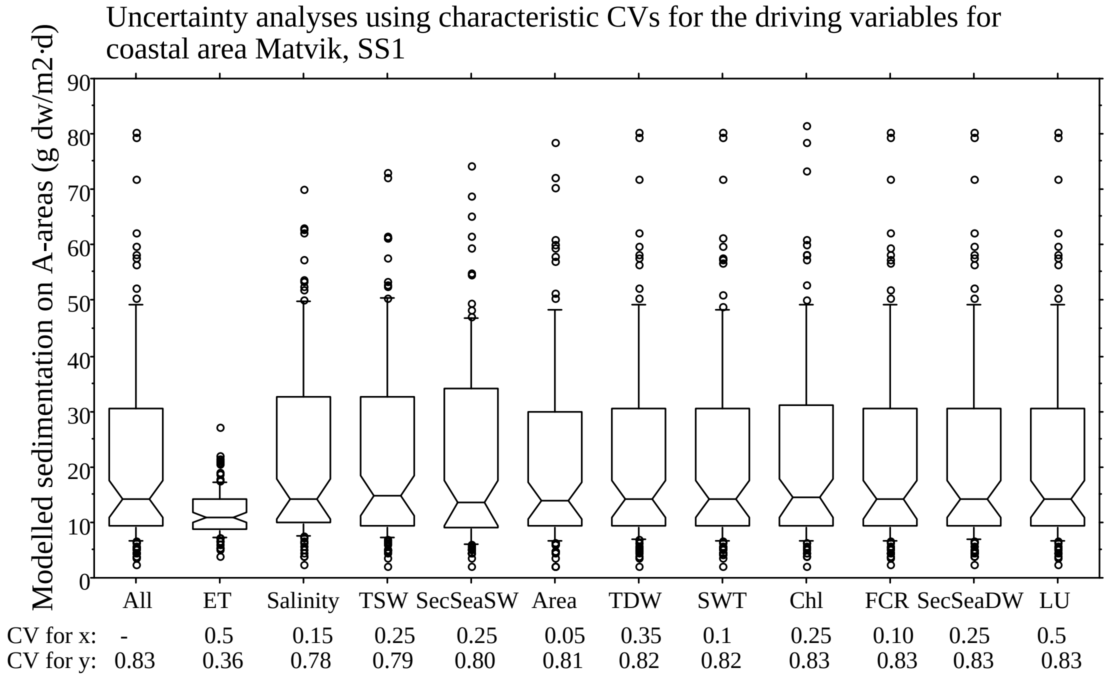

Fig. 12. Frequency distributions for SPM, the particulate concentration (C_{part}), the dissolved concentration (C_{diss}), the particulate fraction (PF) and K_d using the data (n = 52) for the substances given in table 4.

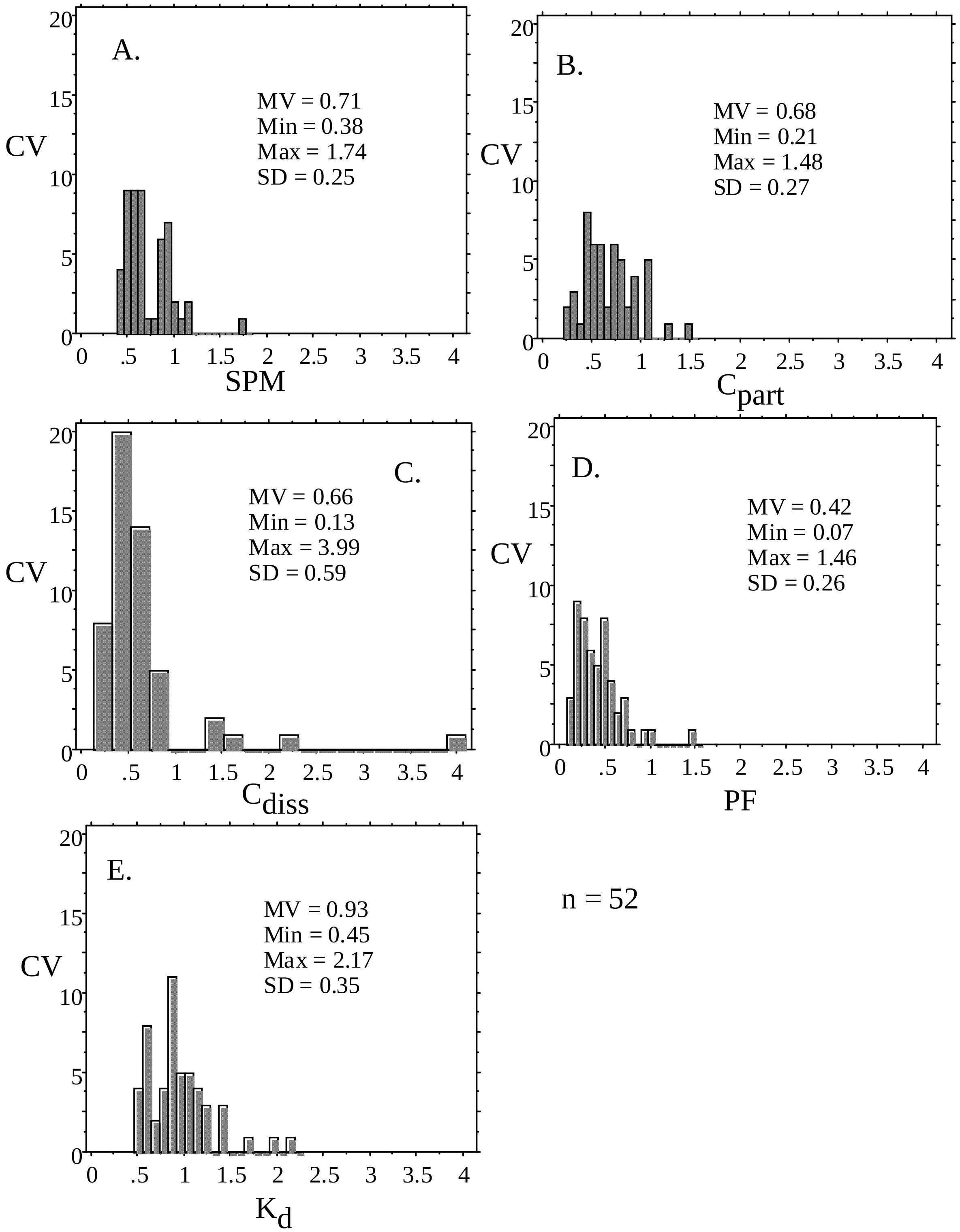

Fig. 13. Test to illustrate that randomly produced parameters can give significant correlations when ratios are being regressed against parameters used in the ratios. Note that all these variables on the y- and x-axes have been produced by a random number generator. The abbreviations are: SPM = suspended particulate matter, C_{part} = particulate concentration, C_{tot} = total concentration, PF = particulate fraction and K_d.

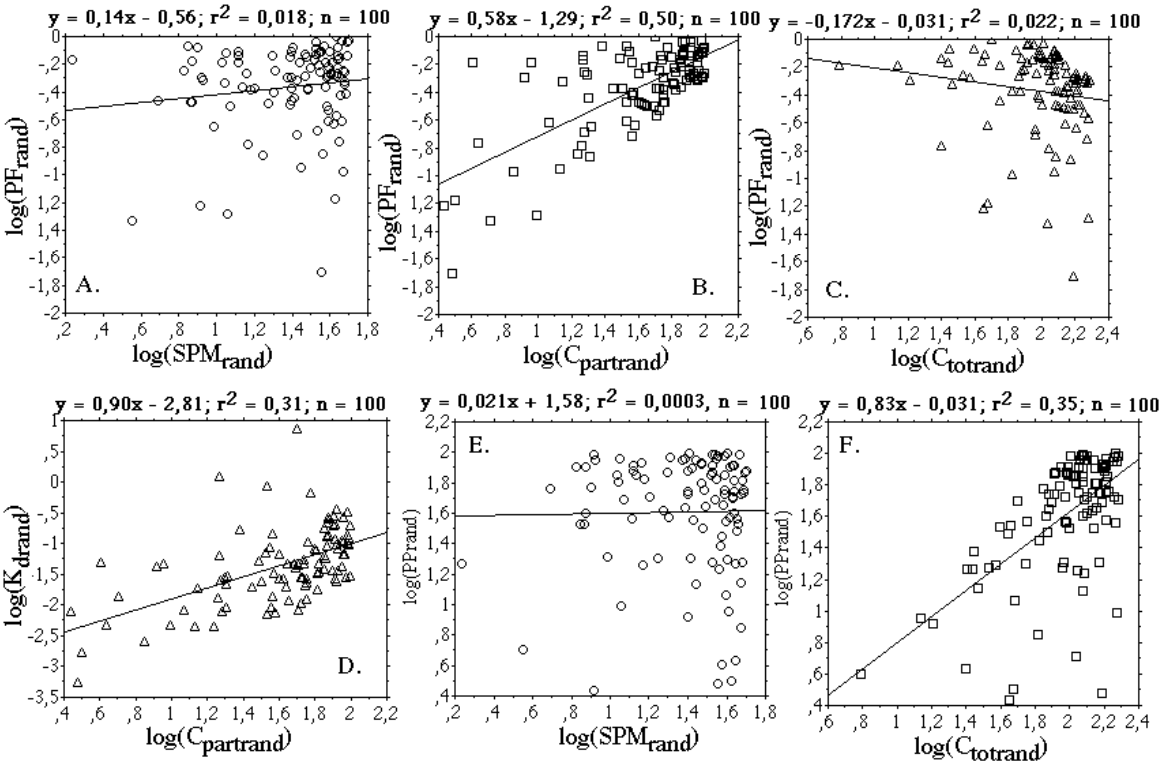

Fig. 14. Illustration of spurious correlations. 1000 data on "water discharge" (Q_{rand}) and "suspended particulate matter" (SPM_{rand}) have been generated and the correlation is shown in fig. C. Fig. A gives the regression between "sediment transport" ($Q_{rand} \cdot SPM_{rand}$) and "water discharge" (Q) for the data in fig. C, and fig. B gives a regression when 10 data-sets like the one in fig. A have been used.

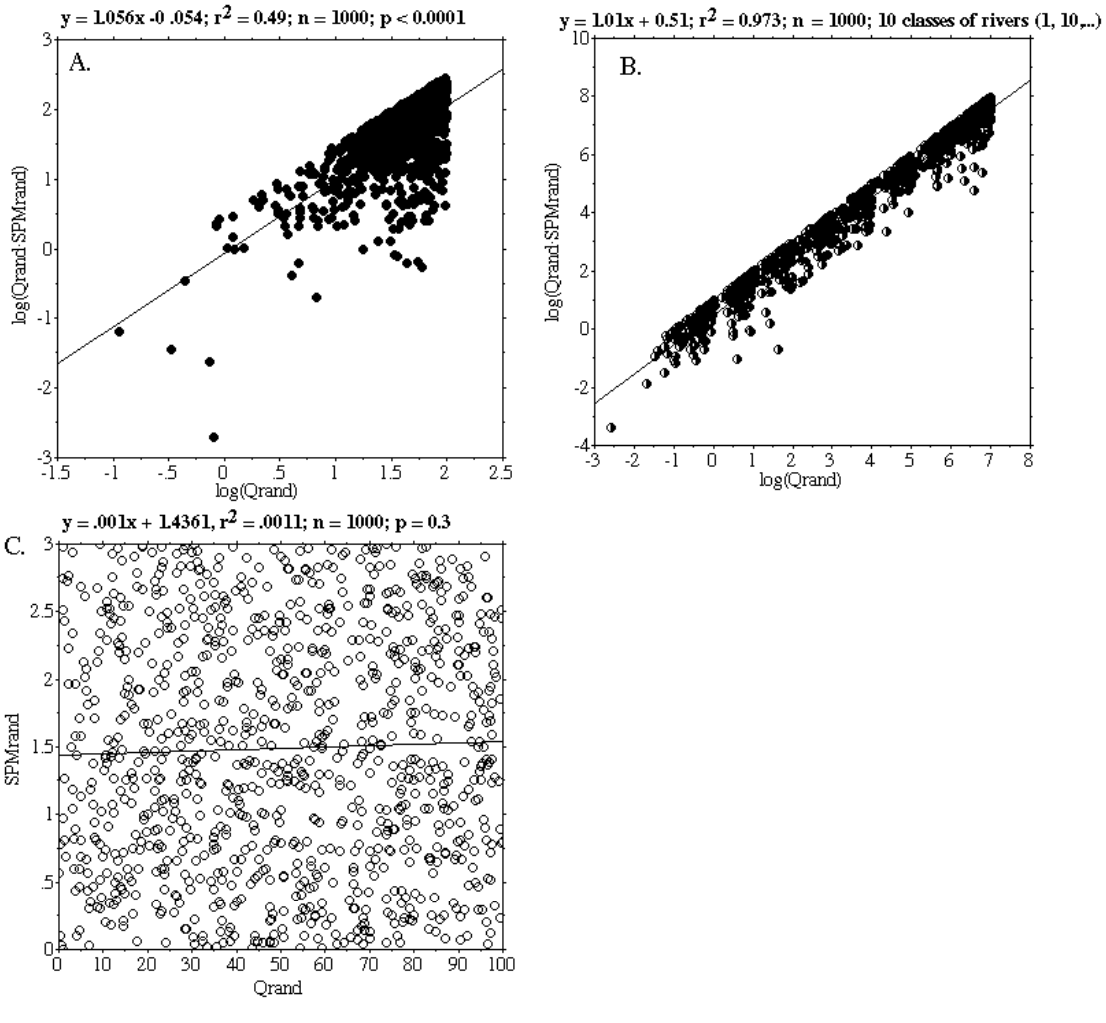

Table 1. Coefficients of within-site or within-system variation (CV) and theoretically highest r^2-values (r_r^2) for variables from (A) sites in an open marine area (the Baltic Sea), (B) marine coastal areas in the Baltic), (C) rivers and (D) lakes. Compilation from Håkanson (2005).

A. Marine open water areas (data from the Baltic Sea; from Håkanson and Eckhell, 2005)		
	CV	$\mathbf{r_r^2}$
SPM	0.67	0.70
Temperature	0.40	0.89
Salinity	0.07	0.997
B. Marine coastal areas (data from Wallin et al., 1992 and Nordvarg, 2001)		
SPM	0.34	0.92
Secchi depth	0.19	0.98
Chlorophyll-a	0.25	0.96
Total-N	0.13	0.99
Inorganic-N	0.31	0.94
Total-P	0.16	0.98
Inorganic-P	0.28	0.95
O_2-concentration	0.26	0.96
O_2-saturation	0.26	0.96
C. Rivers (from Håkanson et al., 2003)		
SPM	1.71	-0.93
Chlorophyll-a	1.15	0.13
Total phosphorus	0.51	0.83
Water discharge	1.42	-0.33
Particulate phosphorus	1.59	-0.67
Dissolved phosphorus	0.77	0.61
Chem. oxygen demand	0.65	0.72
Biol. oxygen demand	0.54	0.81
Conductivity	0.44	0.87
Temperature	0.41	0.89
Particulate fraction of phosphorus	0.31	0.94
Dissolved oxygen	0.25	0.96
Redox potential	0.18	0.98
pH	0.03	1
D. Lakes (from Håkanson and Peters, 1995 and Håkanson, 1999)		
SPM	0.65	0.72
Secchi depth	0.15	0.99
Chlorophyll-a	0.25	0.96
Total phosphorus	0.35	0.92
Alkalinity	0.35	0.92
Fe-concentration	0.25	0.96
K-concentration	0.20	0.97
Colour	0.20	0.97
Ca-concentration	0.12	0.99
Hardness	0.12	0.99
Conductivity	0.10	0.99
pH	0.05	0.998

Table 2. Actual data on SPM-concentrations (mg/l) River Avon (Evesham). Mean values (MV) from 6 samples, the actual data redistributed randomly, mean values of the redistributed data (n = 6). n = number of data, MV = mean values, SD = standard deviations, CV = coefficient of variations and CV/√6.

Actual data	MV, n=6	Random order	MV, rand, n=6		Actual data	MV, n=6	Random order	MV, rand, n=6
13		15			1.5		12	
3		33			1.5		8	
31		16			7		11	
17		12			11		53	
21		13			6		11	
10	15.8	560	108.2		5	5.3	8	17.2
10		3			4		14	
6		67			13		12	
168		5			122		6	
17		4			22		33	
11		10			10		5	
22	39.0	48	22.8		7	29.7	1.5	11.9
14		4			8		10	
560		13			40		8	
165		18			9		16	
67		8			10		22	
36		17			6		13	
53	149.2	15	12.5		7	13.3	14	13.8
21		4			5		10	
13		10			8		13	
33		8			19		18	
12		122			8		168	
18		40			12		13	
48	24.2	31	35.8		10	10.3	1.5	37.3
18		10			8		17	
21		1.5			16		22	
21		12			10		5	
13		7			8		7	
12		7			20		20	
10	15.8	21	9.8		16	13.0	5	12.7
22		10			9		6	
15		12			31		11	
12		165			10		12	
16		10			17		36	
8		9			12		10	
14	14.5	8	35.7		8	14.5	17	15.3
13		6			11		21	
15		31			10		8	
9		6			5		9	
12		5			8		13	
13		19			5		21	
1.5	10.6	22	14.8		9	8	5	12.8
4		9		**n**	90	15	90	15

5		9		**MV**	24.85	24.85	24.85	24.85
4		16		**SD**	63.29	35.50	63.29	24.94
5		10		**CV**	2.55	1.43	2.55	1.00
6		8		**CV/√6**	1.04			
33	9.5	21	12.2					

Table 3. Compilation of characteristic CV-values for different types of aquatic variables (from Håkanson, 1999).

	CV		CV
Morphometric variables		**Sedimentological variables**	
Lake area (Area)	0.01	Percent ET-areas (ET)	0.05
Mean depth (D_m)	0.01	Mean water content for E-areas	0.30
Maximum depth (D_{max})	0.01	Mean water content for T-areas	0.20
Volume (Vol)	0.01	Mean water content for A-areas	0.05
Theoretical water retention time (T_w)	0.10	Mean bulk density for E-areas	0.10
		Mean bulk density for T-areas	0.10
Climatological variables		Mean bulk density for A-areas	0.02
Annual runoff rates	0.10	Mean organic content for E-areas	0.50
Annual precipitation	0.10	Mean organic content for T-areas	0.50
Temperatures	0.20	Mean organic content for A-areas	0.10
		Fall velocities	0.50
		Age of A-sediments	0.50
		Age of ET-sediments	0.50
		Diffusion rates	0.50

Table 4. A compilation of mean-values and coefficients of variation (CV) for particulate concentrations, C_{part} (†), dissolved concentrations, C_{diss} (†), SPM (mg/l), the particulate fraction, PF (-) and K_d ($l/kg^{\cdot}$) for various substances, n = number of data. From Johansson et al. (2001).

Sub-stance	n	Mean					CV					System	Reference*
		C_{part}	C_{diss}	SPM	PF	K_d (10^6)	C_{part}	C_{diss}	SPM	PF	K_d		
Ag^{VIII}	10	5.53	6.21	10.38	0.46	0.14	0.93	0.68	0.69	0.62	0.86	Sabine estuary	1
Ag^{VIII}	5	9.28	5.68	19.70	0.52	0.15	1.26	0.59	0.92	0.37	1.10	Galveston estuary	1
Ag^{VIII}	6	4.00	4.53	17.40	0.58	0.24	0.55	1.45	0.95	0.46	0.82	Colorado estuary	1
Ag^{VIII}	6	1.95	2.45	29.32	0.45	0.050	0.31	0.30	0.98	0.16	0.85	Lavaca estuary	1
Ag^{VIII}	8	5.86	4.58	90.73	0.54	0.019	0.57	0.49	0.38	0.40	0.80	San Antonio est	1
Ag^{VIII}	6	3.75	4.55	26.03	0.46	0.062	0.49	0.52	0.83	0.41	0.75	Corpus Christi est	1
Ag^{IX}	44	118	30.2	10.56	0.74	0.59	0.96	1.53	0.88	0.24	0.86	Quinnipiac River	2
Ag^{IX}	5	6.40	3.80	10.64	0.63	0.19	0.50	0.54	0.47	0.07	0.45	Tivoli South Bay	2
Cd^{V}	9	6.81	12.33	1.27	0.32	0.85	0.90	0.26	0.64	0.72	1.07	Lake Sammamish	3
Cd^{IX}	46	155	68.6	9.96	0.64	0.43	1.08	0.89	0.93	0.29	0.95	Quinnipiac River	2
Cd^{IX}	5	18.8	12.80	10.64	0.61	0.18	0.55	0.86	0.47	0.19	0.59	Tivoli South Bay	2
Cd^{I}	37	0.001	0.013	0.17	0.08	0.63	0.85	0.32	0.49	1.03	1.24	The Baltic Sea	4
Co^{IV}	34	0.27	0.49	1.26	0.61	3.70	0.54	2.21	0.60	0.46	1.45	Lake Sammamish	3
Cr^{II}	40	0.22	1.01	0.99	0.18	0.26	0.65	0.20	0.61	0.59	0.67	Lake Sammamish	3
Cu^{IV}	46	1.08	5.82	1.15	0.17	0.19	0.59	0.24	0.46	0.74	0.62	Lake Sammamish	3
Cu^{VII}	13	0.16	0.97	10.51	0.17	0.025	0.69	0.56	0.57	0.74	0.78	Sabine estuary	1
Cu^{VII}	16	0.24	0.94	12.96	0.21	0.034	0.74	0.33	0.91	0.63	0.93	Galveston estuary	1
Cu^{VII}	12	0.13	0.90	13.47	0.12	0.018	0.87	0.23	0.92	0.56	0.88	Colorado estuary	1
Cu^{VII}	13	0.14	0.79	19.58	0.16	0.022	0.81	0.52	1.07	0.77	1.24	Lavaca estuary	1
Cu^{VII}	14	0.21	1.08	66.23	0.16	0.003	0.71	0.40	0.59	0.52	0.50	San Antonio est	1
Cu^{VII}	13	0.23	0.86	24.55	0.23	0.015	0.41	0.49	0.56	0.40	0.56	Corpus Christi est	1
Cu^{I}	37	0.013	0.387	0.17	0.06	0.43	0.74	0.42	0.49	1.46	1.39	The Baltic Sea	4
Mn^{I}	18	8.41	67.6	0.15	0.53	20.8	1.48	3.99	0.67	0.51	1.19	The Baltic Sea	4
Ni^{IV}	40	0.52	4.88	1.53	0.09	0.09	0.93	0.25	0.62	0.92	1.14	Lake Sammamish	3
P^{I}	17	5.35	3.71	1.13	0.62	2.49	0.27	0.68	0.39	0.28	1.04	Lake Njupfatet	7
P^{I}	11	26.7	28.31	6.35	0.52	0.26	0.28	0.44	0.83	0.20	0.45	Lake Björkaren	7
P^{I}	19	47.5	28.32	12.02	0.60	0.22	0.71	0.49	1.00	0.19	0.68	Lake Kundby	7
P^{I}	27	7.33	5.19	1.07	0.58	2.71	0.45	0.56	0.51	0.35	1.17	Lake Siggefora	7
P^{I}	63	11.1	13.72	2.39	0.47	0.62	0.42	0.53	0.47	0.20	1.38	Lake Erken	7
P^{I}	18	7.39	12.22	1.71	0.37	0.49	0.33	0.13	0.82	0.18	0.57	Lake Örträsket	7
Pb^{II}	66	0.25	0.07	1.28	0.71	4.97	0.56	0.62	0.60	0.17	0.82	Lake Sammamish	5
Pb^{VII}	16	0.16	0.09	11.36	0.60	0.26	0.80	0.73	0.55	0.32	1.06	Sabine estuary	1
Pb^{VII}	16	0.20	0.07	12.93	0.65	0.32	0.81	0.41	0.91	0.32	1.01	Galveston est	1
Pb^{VII}	12	0.17	0.07	10.48	0.69	0.75	0.66	0.49	0.49	0.24	2.17	Colorado estuary	1
Pb^{VII}	13	0.11	0.07	18.62	0.56	0.13	1.07	0.46	1.14	0.30	0.82	Lavaca estuary	1
Pb^{VII}	15	0.15	0.10	63.31	0.62	0.047	0.42	0.69	0.62	0.25	0.85	San Antonio est	1
Pb^{VII}	13	0.15	0.08	24.55	0.55	0.10	1.10	0.63	0.56	0.49	0.88	Corpus Christi est	1
Pb^{IX}	51	1091	155.1	10.35	0.80	1.15	0.79	0.63	0.89	0.25	0.91	Quinnipiac River	2
Pb^{IX}	13	446	96.2	7.15	0.81	1.02	0.47	0.50	0.60	0.12	0.73	Tivoli South Bay	2
Pb^{IX}	21	17.7	12.1	0.48	0.60	11.77	0.57	0.91	1.74	0.32	0.90	Bear Brook	2
Pb^{I}	37	0.008	0.020	0.17	0.33	5.07	0.49	0.70	0.49	0.50	1.03	The Baltic Sea	4
$^{210}Pb^{III}$	61	2.46	0.68	1.43	0.75	6.08	1.04	1.33	0.59	0.26	1.11	Lake Sammamish	5
$^{210}Pb^{VI}$	20	3.68	1.89	0.68	0.65	3.69	0.42	0.47	0.43	0.21	0.58	Lake Crystal	6
$^{210}Po^{III}$	59	0.89	0.54	1.44	0.64	2.13	0.44	0.63	0.59	0.24	1.64	Lake Sammamish	5
$^{210}Po^{VI}$	20	3.07	1.08	0.68	0.75	5.56	0.21	0.42	0.43	0.09	0.48	Lake Crystal	6
Zn^{II}	8	1.06	3.35	1.25	0.26	0.51	0.46	0.36	0.78	0.56	0.99	Lake Sammamish	3
Zn^{VII}	14	0.66	1.16	11.75	0.34	0.055	0.80	0.43	0.55	0.49	0.60	Sabine estuary	1
Zn^{VII}	14	1.59	1.85	13.65	0.43	0.11	1.07	0.63	0.91	0.45	0.98	Galveston estuary	1
Zn^{VII}	13	0.78	0.98	13.46	0.45	0.098	0.44	0.38	0.88	0.35	0.57	Colorado estuary	1
Zn^{VII}	13	1.22	1.72	18.62	0.44	0.086	0.60	0.74	1.14	0.42	0.87	Lavaca estuary	1
Zn^{VII}	15	1.38	0.83	63.31	0.60	0.034	0.60	0.34	0.62	0.17	0.58	San Antonio est	1
Zn^{VII}	13	4.27	3.15	24.55	0.53	0.14	0.74	0.51	0.56	0.46	1.96	Corpus Christi est	1

† Concentrations in: I = µg/l; II = nM; III = dpm 100 per l; IV = nmol/kg; V = pmol/kg; VI = pCi/100l; VII = ppb; VIII = ppt; IX = ng/l.
* 1 = Data from Benoit et al., 1994; 2 = Data from Benoit, 1995; 3 = Data from Balistrieri et al., 1992; 4 = Data from Pohl and Hennings, 1999; 5 = Data from Balistrieri et al., 1995; 6 = Data from Talbot and Andren, 1984; 7 = Håkanson and Johansson (not published)