4 Applications of the SIA-Method: Variability of Mass Fluxes under Field Conditions and Summary of Nitrate Losses under different Land Uses.

4.1 Introduction

The heterogeneity of mass fluxes in the soil is a very well known phenomenon (Beven and German 1982; Jury and Flühler 1992; Netto 1999) and preferential flow has been shown to be important especially in agricultural fields (Williams et al. 2003) and regardless of soil structure and texture (Wang et al. 2003).

The problem of mass flux heterogeneity has been approached from three sides. Undisturbed or disturbed soil columns have been used in the laboratory to measure breakthrough curves of different tracers and water with high time and space resolutions (Zurmühl, Durner, and Hermann 1991; Saxena, Jarvis, and Bergstrom 1994; Chendorain and Ghodrati 1999). Lysimeters, suction cups, TDR, tensiometers, soil coring and drainages have been used to sample from mass fluxes in the field (see chapters 2, 3). Several theoretical approaches such as probability density functions, convection-dispersion models and models taking into account sorption, biodegradation or two-site two-region models have been used to evaluate the empirical findings (Lilburne and Webb 2002; Jury and Flühler 1992; Roth et al. 1991; Paramasivam et al. 2002; Ren, Ma, and Zhang 2003).

Even though heterogeneity is a well known problem, little information exists on its importance and spatial distribution under varying conditions (Onsoy et al. 2005).

It is now widely agreed that a description of mass transport by model or by measurement has to account for the processes matrix flux, preferential flow, particulate transport, sorption (maybe with varying affinities) and degradation (depending on solute). This may be done explicitly by measuring / modelling these processes directly or implicitly, e.g. by using statistical approaches, ‘lumped’ variables or effects.

All methods other than soil coring (e.g. Onsoy et al. 2005) have not been used extensively to gather large sample sizes, which give information about field heterogeneity. But soil cores have mostly been used to measure material properties or state variables like Corg- content, texture, actual water content and more rarely for transport objectives, which require regular sampling. The main drawback of these studies is that no information is available on the time between two samplings and e.g. preferential flows may have passed by unnoticed.

The Self-Integrating Accumulator (SIA)-method has found widespread application in applied field experiments. A set of 3048 data exists for nitrate – losses under field conditions (Bischoff, unpublished). Since the SIA method has been shown to represent the water fluxes under field conditions (cf. chapter 2) adequately, these data may be a valuable source of information on diffuse leaching / mass transport under agricultural fields.

Nitrate movement is a good indicator for water fluxes (Cameron and Wild 1982; Williams et al. 2003; Clay et al. 2004), because the sorption of anions like nitrate or chloride is generally very limited under temperate region conditions.

Objectives

A large data set (N = 3048) of N-losses is analysed. Typical values and variation for different land uses are shown. A concept is developed to use these nitrate-leaching data to evaluate mass transport in the soil in general. The influence of scale and season on the heterogeneity of mass fluxes in soils is assessed.

4.2 Materials and Methods

4.2.1 General

The data set presented here consists of 3048 nitrate loss measurements made in a period of seven years on 47 different fields with about 120 treatments mainly situated in Germany. Most of the studies were performed on private farmers fields under their practical management conditions. The available field information is often very limited. Therefore, the analysis in this paper will be limited to aspects, which do not need assumptions with regard to field properties. Also, the fields may have different measurement replications and / or sampling periods. In general, though, there were 10 replicate nitrate measurements per treatment or field. Treatments included soil management, fertilizers, pesticide application, plant species and others, all of which will not be used as relevant information in this paper, but had to be considered in the choice of data sets included in this analysis.

4.2.2 Sites

The location of the field sites and their regional attribution can be seen in Figure 4-1:

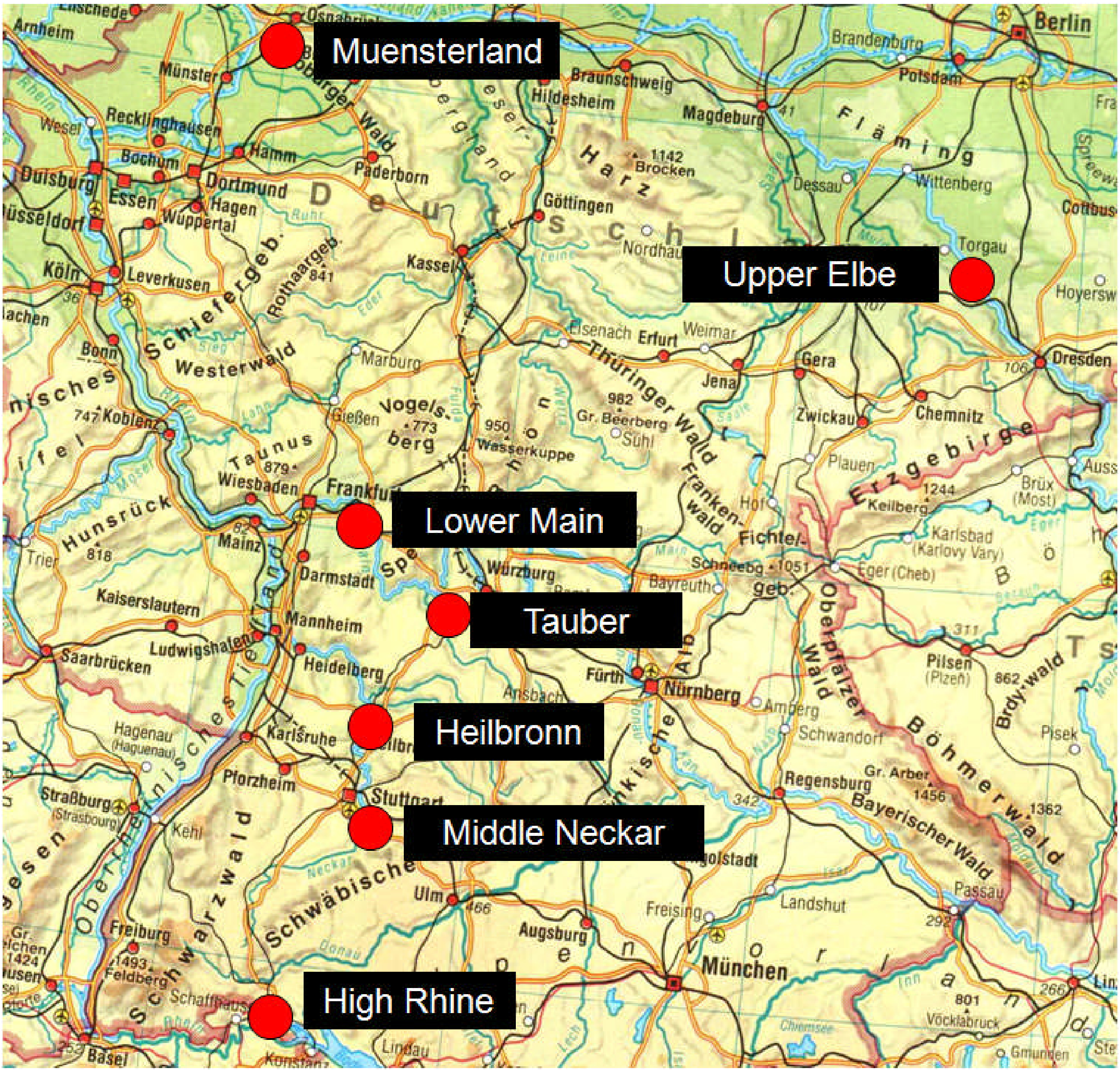

Figure 4-1: Location of the regions with at least three independent fields

SIA have been installed in 47 fields with at least 10 replicates. 44 of 47 fields have been attributed to 7 regions, each containing at least 3 separate fields. The other three fields (two fields near Bern, Switzerland, one close to Karlsruhe) were included in all other scale analyses.

4.2.3 Measurements

The SIA method has been described in more detail in chapters 2 and 3.The SIA were mostly installed in 3 profiles containing 3, 4 and 3 replicates or in 2 profiles with 5 replicates each at depths of either 60, 90, or 100 cm. The experimental setup depended on the objectives of the different studies, but the SIA were always below the main root zone of the crops.

In general, the SIA were installed for a sixth months period (April to September / October to March) and exchanged directly for the consecutive measurements until the end of the studies ranging from sixth month (2 fields) to 6 years (4 fields) with the bulk of the fields between 2-3 consecutive years (4 – 6 measurement periods).

The October to March period will be regarded as a period, where water flow and leaching occur in a major part of the period. and called ‘Winter’.

The April to September period will be regarded as a period, where downward water flow in greater depths does not necessarily occur and cannot be explained by a surplus of the water balance at least in normal and dry years. It will be called ‘Summer’.

Slight deviations from these general conditions have occurred in some cases, but the cases have been included, when they where in general agreement with the conditions set up in this section.

The installation and measurement of the nitrate-N fluxes are described in chapter 2.

4.2.4 Nitrate – general flux transfer function

A way had to be found to extract the information of water fluxes from the combined information of water flux and nitrate concentration implicit in the SIA measurement. At the same time, different scales and times had to be made comparable.

Therefore, two variables were generated to derive a general flux transfer function. One generic variable is the normalized Mass Flux (MF), which is defined as:

$MF = NL / FM$ **(eq. 1)**

where NL is the Nitrate-N Loss [$kg*ha^{-1}$] measured by one SIA and FM is the Field Mean of all Nitrate Losses [$kg*ha^{-1}$] on the same field in the same measurement period.

The second variable is the normalized Absolute Difference (AD) between the Field Mean and the SIA measurement, defined as:

$AD = \mathrm{ABS}\ (MF - 1)$ **(eq. 2)** with ABS = absolute value

The first variable is needed for the comparability of all measurements, when the nitrate-N level differences are cut out and only their variability prevails, which represents the variability of water fluxes, as will be discussed below. The second variable is needed to have a measure of heterogeneity with a spread in the means at different subsamples, which can be tested statistically by an analysis of variance.

For both variables, also the $\log_{10}$ written as lg was calculated, because - as the original data – they were supposed not to be distributed normally.

4.2.5 Test for (Log)Normal Distribution

All variables NL, MF, AD and their $\log_{10}$ values were tested for normality and found to be distributed strictly NOT normal. Therefore, parametric statistical analysis is only allowed at $N > 30$ for any subgroup following the central limit theorem. In other cases, non-parametric statistics have to be used.

4.2.6 Statistical design

The nitrate-N losses were analysed for differences in land use (agriculture, grocery, forest) and season. Means, standard deviations and an analysis of variance was performed. Due to the high replicate N, a parametric "Tukey Honest Significant Difference" post hoc comparison test (Tukey HSD) for samples with unequal N could be performed, but the results are also supported by a "Kruskal-Wallis" rank analysis of Variance, which is not dependent on normal distribution.

The mass flux and heterogeneity variables MF, AD data set was analysed using means, standard deviations (Std. Dev.), coefficients of variation (CV = Std. Dev. / Mean), "Tukey HSD" and "Kruskal-Wallis" analysis of variance using the "Statistica" software package.

The analysis was applied within the scale categories Total, Region , Field, Profile and the water regime categories Summer and Winter. The largest distances for the different scales between the SIA measurements were > 500 km (total), < 30 km (region), < 500 m (field) and < 1 m (profile).

In addition, correlations between Summer and Winter CV were calculated with linear regression analysis.

4.3 Results and Discussion

4.3.1 Nitrate losses under different land uses

The summary of the total data set (Figure 4-2) shows that leaching occurs mainly in the period between October – March under German conditions and is strongly dependent on land use. Intensive vegetable production requires high fertilizer inputs for premium quality to be competitive on the German grocery market at the moment. Also, the cultures are harvested selectively in grocery. Plants, which do not meet the market standards, are left on the fields. Harvest efficiency was in the range of 70 % in the studies, but total failures with no harvest occurred. Therefore, grocery accounts for the biggest nitrate-N losses per year with a mean of 120 kg*ha^{-1}, agricultural losses are in the range of 43 kg*ha^{-1} and forest merely looses about 8 kg*ha^{-1}.

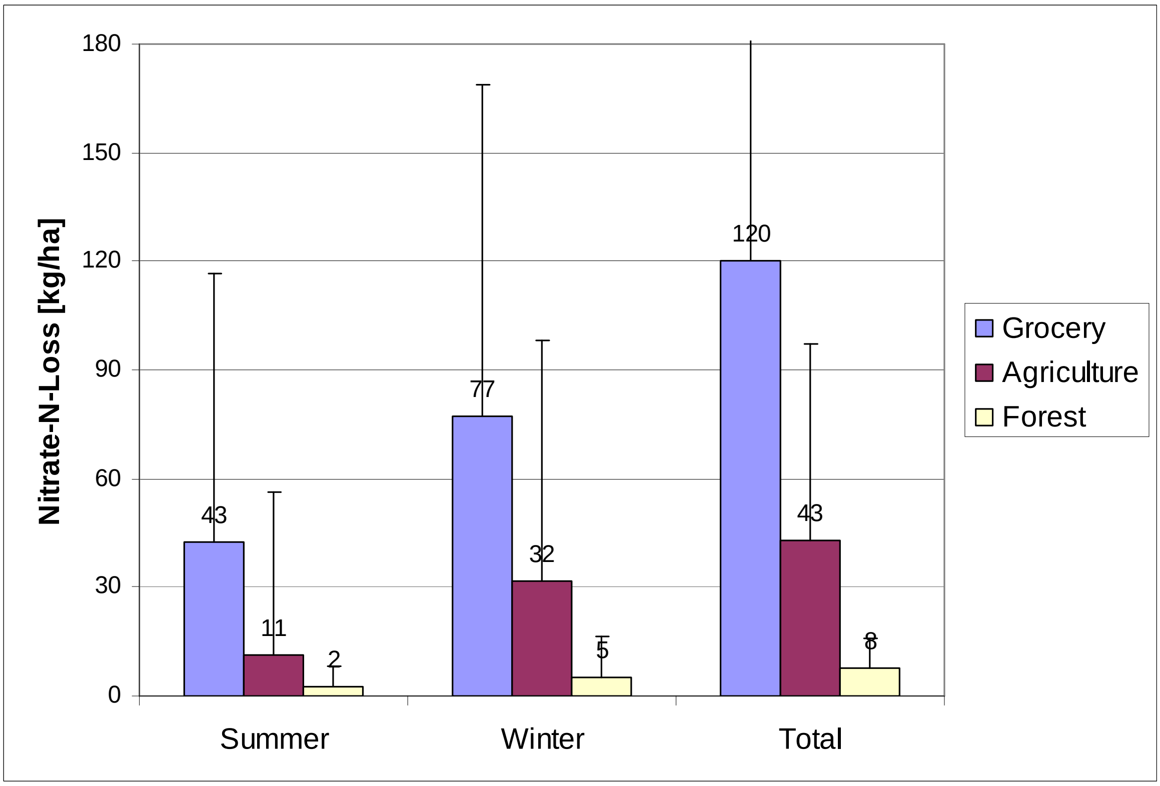

*Figure 4-2: Nitrate-N losses [kg*ha^{-1}] under different land uses and their variability. Error bars = Std. Dev.. Total N = 3048.*

'Summer' leaching, which in our definition may include some leaching in spring accounts for 26 % (Agriculture), 32 % (Forest) and 36 % (Grocery) of the total losses. The higher proportion in grocery can be explained by a higher proportion of irrigation.

The variation is large and ranges between a CV of 118 % for Grocery in the winter time and 406 % for agriculture in the summer. Part of the variation can be attributed to management practices and fertilization, but another part will be strongly dependent on leaching- and mineralization- conditions.

4.3.2 Nitrate as a tracer for water fluxes

4.3.2.1 Water flux variability represented by nitrate data: Mathematical derivation and discussion

The amount of Nitrate-N losses $N_{total,\ SIA}$ [kg*ha^{-1}] in one measurement with the SIA method can be seen as:

$$\int_{t1}^{t2} (WA(t) * Nconc.(t))dt = N_{total,SIA} \quad \textbf{(eq. 3)}$$

, where WA(t) is the water rate leached [L*ha^{-1}*a^{-1}] and Nconc.(t) is the nitrate-N concentration [kg*L^{-1}]. For our objective it is sufficient to extract a variable which is proportional to the integral of WA. It need not be the correct value of WA itself, because every variable proportional to WA by a constant factor contains the same information about the variability in space and time.

It can be assumed that the variability with time of Nconc. can be neglected because of large repetition numbers, which cancel out these effects. In addition, these effects are partly filtered by the normalization procedure: At the field scale periods of high and low Nitrate-N availability are the same for every data point in the same season, because the most important factors management, soil and weather are very similar.

Therefore, under the assumption that the variation of Nconc.(t) is extracted in the procedure of normalization, **eq. 3** reduces to:

$$\int_{t1}^{t2} WA_n(t) * dt = WA_n = \frac{k * N_{total,SIA}}{\mu_{Field}(N_{total,SIA})} \quad \textbf{(eq. 4)}$$

,where WA_n is the total water amount [l*ha^{-1}] which passed through the nth SIA replicate during the measurement period, μ_{Field} is the mean total N loss [kg*ha^{-1}] on that field in that season and k is a proportionality factor [l*ha^{-1}].

Nitrate has some properties, which are favourable to use it as a water transport tracer:

It is ubiquitous in (aerobic) agricultural fields. On the field scale, it is rather uniformly released from fertilizers and the organic substance to the soil solution in space, though not in time. Nitrate is a non-sorbing solute, which behaves as a conservative tracer in the absence of biotic uptake or biodegradation. Nitrate has already been used by (Williams et al. 2003) as a tracer in preferential flow path experiments to show spatial variability in a lysimeter study. There was no difference in rates of movement between chloride and nitrate in a comparison study (Cameron and Wild 1982).

In contrast, (Clay et al. 2004) found a difference between bromide and nitrate breakthrough in soil column experiments. This was attributed to immobilization, denitrification or less anion exclusion. Therefore, the difference is due to chemical and not transport dynamics. The concentration levels vary during the year and between years due to plant and soil biological activity, which in turn depend mainly on water content, temperature and growth stage and therefore in a first approximation on the season. Fertilization and soil management are the main anthropogenic influence factors (Zhu, Fox, and Toth 2003; Grigg et al. 2004; Martin et al. 2004; Korsaeth, Bakken, and Riley 2003).

It is reasonable for this analysis that short term effects like mineralisation and immobilisation phases, which have to be taken into account, if samples are taken intermittently, will not influence the comparability of the results, because these effects are fully covered by the integrative measurement by the SIA over a six month period.

Also, it is reasoned that the nitrate sources humic substance, plant residue and fertilizer are distributed evenly over one field or treatment. Most of the fields have been carefully chosen to compare different treatments on comparable soil adjacent to each other. It adds to the plausibility that small inhomogeneities in the top soil may also be mixed during the passage through the root zone towards the SIA. Therefore, the nitrate source is supposed to be homogeneous with regard to the field scale.

One bias to the data with regard to water fluxes is inherent and can not be extracted with the standardization method. The variation of Nitrate-N source strength is a weighting factor for the water flux at the same time. This may emphasize water fluxes in times of high Nitrate-N availability *during the same measurement period* in the results. It does not influence the comparability between samples from different fields or years, but may be an error within the one standardized field + season data set of 10 replicates. Because of the large overall data set it can be reasoned that these time dependent effects will be negligible for subsamples with high replicate numbers (N), which cover several fields and time periods. This is true for all shown subsamples but the Muenster region, which only covers two seasons in one year.

Therefore, it is concluded that for this data set Nitrate-N can be used as a tracer for integrated mass fluxes with some limitations.

4.3.2.2 Variability calculation results and discussion

The heterogeneity as generalized information can best be represented by the coefficient of variation (CV) at the respective scale and its variability between the subsamples (Table 4-1). The mean CV at the profile scale with distances of 0,1 – 1 m between the SIA is in the range of 62 % (Range: 11 - 186 %, Std.Dev.: 29 %) in winter time and 104 % (Range: 23 – 300 %; Std.Dev.: 52 %) in summer time for all 207 profiles.

Table 4-1: Summary table of heterogeneity expressed as the normalized coefficient of variation (CV [%]) and its corresponding standard deviations (Std.Dev.) with respect to scale (rows) and season (columns).

	CV Winter	**CV Summer**	Std.Dev. Winter	Std.Dev. Summer	Summer/ Winter
Profile	62%	104%	29%	52%	167%
Field	80%	135%	23%	53%	169%
Region	99%	132%	14%	20%	133%
Total	93%	135%			145%

The heterogeneity increases at the field scale, where CV mean values are 80 % (Range: 41 - 135 %, Std.Dev.: 23 %) in winter time and 135 % (Range: 63 – 317 %; Std.Dev.: 52 %) in summer time for all 47 fields.

Figure 4-3 shows the variation of water fluxes within and between the 7 German regions. The heterogeneity at the regional scale is still higher than at the field scale for the winter period with a mean CV of 99 % (Range: 70 - 114 %, Std. Dev.: 14 %). For the summer the mean CV is more or less the same with 132 % (Range: 103 - 159 %; Std. Dev.: 20 %). But the variation between the CVs of different regions is markedly lower than between different fields or plots.

Significant differences between the regions were found between the Lower Main region with high regional variability (Winter CV: 114) and the High Rhine, Tauber and

Middle Neckar with winter CVs of 97, 96, 70 % respectively by Tukey HSD and Kruskal-Wallis Analysis.

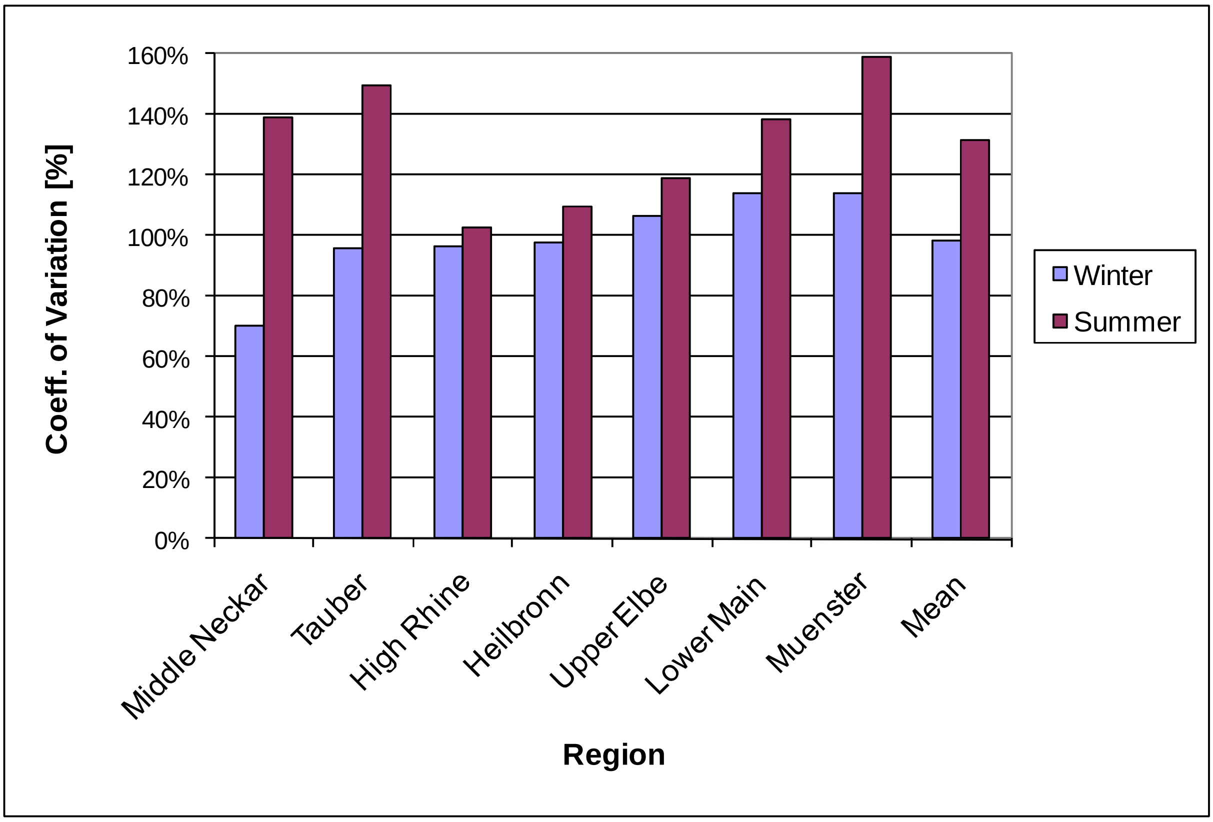

Figure 4-3: Variation of nitrate fluxes within and between the 7 German regions

A graphical summary about the heterogeneity of water fluxes at different scales is given in Figure 4-4 (below). It shows that in the winter months the heterogeneity increases with increasing scale to the level of the region, whereas the variability between subsamples decreases at larger scales. This is to be expected, because the variation should increase with differences in soils and soil management.

The decrease in heterogeneity above the regional scale is due to the inconsistency of data in the statistical analysis. At the regional scale, samples, which could not be grouped into one region, had to be excluded from the analysis. This included larger data sets from 3 fields with several years of measurement with CVs between 60 – 70 %, which had to be taken into the total sample, because they were used for analysis at the profile and field scale. Without them, the interregional CV increases to about 100 % and is not significantly different from the regional CV.

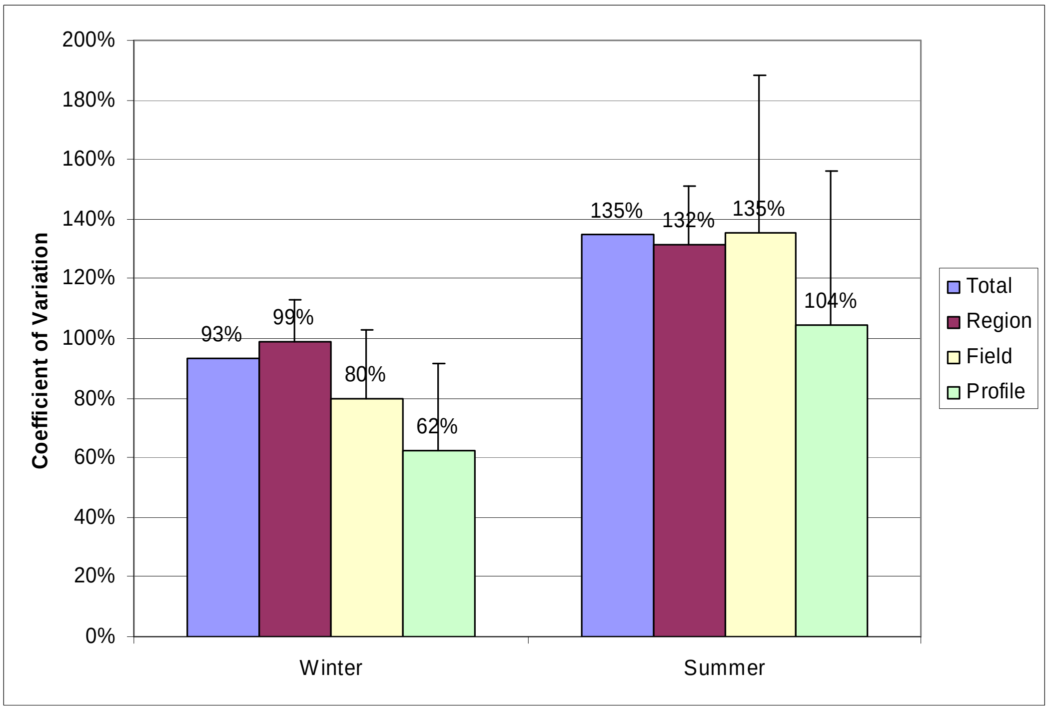

Figure 4-4: Summary about the heterogeneity of water fluxes at different scales. Heterogeneity expressed as coefficient of variation (CV [%]). Error Bars = Standard Deviation

From these results, the extent of variation in water fluxes at every scale is now established.

The summer water flux heterogeneity is always significantly higher than in winter and increases significantly only up to the field scale. The variation between subsamples at the same scale expressed as standard deviations decreases. The heterogeneity of summer fluxes is 30 – 60 % higher than that of winter fluxes.

This increase in heterogeneity during the summer months can be attributed to differences in the flow regime. In winter the soils are normally saturated to field capacity and flow occurs in the whole range of the pores, but is dominated by pores with high hydraulic conductivity.

In summer the soil is typically unsaturated under German conditions and may be very dry. Flow occurs only through very big structures like dry cracks, earthworm holes etc., when heavy rainfall events may exceed the infiltration capacity. An example for preferential flow has already been evaluated in Chapter 2. The example showed that the variability in summer is not only a function of the secondary structure of the soil, but also of the rainfall distribution and intensity, which contribute to yes/no flow conditions.

To conclude, the main effect for higher variability in the Summer is the intermittent and area restricted or ‘hot spot’ flow regime.

As a consequence, it seems appropriate that summer measurements need more measurement replications for the same error in the estimate. Assuming a normal distribution, which unfortunately doesn’t seem to be the case for mass fluxes in the soil, 10 replicates would be sufficient for an error estimate of 25 % in winter but only 43 % in summer.

This may be acceptable for practical purposes, because the summer losses account only for about 30 % of the total losses in nitrate-N. The proportion of water lost during this period is probably far below this, but the concentrations of nitrate-N are higher in summer.

From these results, the high variation in water fluxes is now established and quantified at different scales. The assumption of homogeneous soil conditions = homogeneous mass fluxes is only valid including a good proportion of chance error. But the extent of the error should be known: From our point of view, these data provide the means to make field heterogeneity something to calculate with. I have given typical values and ranges for several scales relevant to field research. I strongly support the view that results from transport experiments in the field are only valid, if variation due to heterogeneity is accounted for and can be separated from variation due to treatment.

4.3.2.3 Influence of the sample scale

From the discussion about the correct size of a representative elementary volume of soil, which is required to get ‘typical’ results for ‘the whole’ homogeneous field, it seems obvious that the catchment / sampling area of the field method may influence the variability of the data. It could be expected that bigger areas may show lower variability. But it could also be argued that there is a lower limit to effective sampling. I suggest that it would be in the range of the ‘typical’ aggregate size / macropore spacing, because the secondary structure and biopores provide the highest hydraulic conductivities in the soils. Therefore, they are generally speaking responsible for most of the downward mass fluxes.

With regard to our study the question can rest unanswered, because a) the evaluation is valid for everyone using this method and b) most other methods used in the field have catchments / sampling areas of the same dimension. However, it rests to show, if with a given sampling area a few bigger or many smaller samples /devices are better suitable to represent a visually homogeneous field.

4.4 Summarizing remarks and conclusions

The results from the SIA method demonstrated that land use strongly affects Nitrate-N losses under practical conditions. Within similar land uses the spread of Nitrate-N losses is high, so there is a potential for better management practices. The SIA method can be used as an efficiency control to compare management strategies.

A simple mathematical method was derived and discussed to calculate and evaluate field heterogeneity of mass fluxes from integrated Nitrate-N loss measurements. The method seems appropriate to use nitrate as a water flux tracer with some limitations.

The results show a large heterogeneity of water fluxes within the soil. The heterogeneity increases with scale from a mean CV of 60 % within a soil profile to 100 % within and between regions. This means that the Standard Deviation for Mass Fluxes is close to or higher than the measured mean. Many sample replicates are therefore required to get sound results with an acceptable error in the mean estimate.

Seasonal variations influence the variability of fluxes due to the changes in the water flow regime.

This analysis provides good first information for the planning of scientific transport experiments, because it includes heterogeneity due to scale and season on a broad data set under practical field conditions. It can be a reference for the planning of the amount of replications needed for transport experiments at the field scale.

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