Uncertainty analysis at large scales: limitations and subjectivity of current practices - a water quality case study

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Abstract Uncertainty analysis for large-scale model studies is a challenging activity that requires a different approach to uncertainty analysis at a smaller scale. However, in river basin studies, the practice of uncertainty analysis at a large scale is mostly derived from practice at a small scale. The limitations and inherent subjectivity of some current practices and assumptions are identified, based on the results of a quantitative uncertainty analysis exploring the effects of input data and parameter uncertainty on surface water nutrient concentration. We show that: (i) although the results from small- scale sensitivity analysis are often applied at larger scales, this is not always valid; (ii) the current restriction of the uncertainty assessment to uncertainty types with a strong evidence base gives structurally conservative estimates; (iii) uncertainty due to bias is usually not assessed, but it may easily outweigh the effects of variability; (iv) the uncertainty bandwidth may increase for higher aggregation levels, although the opposite is the standard assumption.

Keywords Modeling; scale; subjectivity; uncertainty; water quality

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Introduction

Information about uncertainty is generally held to improve the quality of decision making; it adds a useful dimension by revealing the reliability of the knowledge produced. Different methods for classification of uncertainty have been presented (see e.g. Morgan and Henrion, 1990; van Asselt *et al.*, 2001; Walker *et al.*, 2003), but there is no generally agreed classification. The comprehensive classification of Walker *et al.* (2003), originating from model-based decision support, distinguishes four sources of uncertainty leading to model outcome uncertainty: input data, parameters, model and context. This paper is restricted to considering uncertainty in input data and parameters. Although the benefit of uncertainty analysis is widely recognized in the scientific community, in practice uncertainty analysis is not common. One of the reasons is that uncertainty analysis is still seen as difficult to perform, partly because of a lack of clear guidance (Pappenberger and Beven, 2006). Over recent decades, guidelines, methods and overviews of methods have been published for dealing with uncertainties, in particular input data and parameter uncertainties (e.g. Yoe and Skaggs, 1997; van der Sluijs *et al.*, 2003; Floodrisknet, 2007). However, translating these methods to the level of practical application is still a challenge in environmental science and other fields. Difficulties arise for analyses at larger (e.g. catchment) scale, as both the availability of uncertainty data and model development and testing often take place on a small scale (Heuvelink and Pebesma, 1999). For large-scale analysis, information on uncertainty needs to be upscaled. Moreover, other sources and types of

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uncertainty may become important (Beven, 1995). This involves choices about which methods to apply and which uncertainties to include in the analysis. In current uncertainty analysis at large scales, the following approaches are common practice: (i) the important uncertainty sources for larger scale analysis are often selected based on sensitivity analysis and expert judgment on small scale; (ii) uncertainty analysis focuses on the uncertainty sources for which clear evidence exists, following a mainly data-driven approach; (iii) uncertainty assessment is focused on uncertainty which is due to variability - often neglecting uncertainty due to bias; (iv) uncertainty bandwidths are, as a rule, assumed to reduce with an increasing aggregation level of the output variable. These common practices are mostly derived from existing practices at small scales. In this paper, their validity is tested at a larger scale, using an uncertainty analysis modeling case study.

Methods

To test the validity of the four common practices introduced in the previous section, four experiments were performed for an uncertainty analysis case study.

- The selection of uncertainty sources was based on sensitivity analysis and expert judgment on a small scale, and was then used in the case study on a catchment scale. One uncertainty source is selected to test the validity of this approach.
- For one uncertainty source, uncertainty types were included for which no clear evidence exists for their existence or magnitude; expert judgement was used for their assessment. This approach is compared to an assessment restricted to evidence-based uncertainty types.
- For one uncertainty source, uncertainty due to bias was included. The effect of uncertainty due to bias is compared to the uncertainty due to variability.
- In the analysis of the results, different spatial and temporal aggregation levels of the output were collected to see the influence on the uncertainty bandwidth.

Application: a case study

The influence of input data and parameter uncertainty related to diffuse emissions on the summer averaged phosphorus and nitrogen concentrations at the outlet of the Regge river catchment was analyzed for 1999.The analysis is methodological and was not carried out with the intention of providing direct decision support; only a selection of uncertainties was assessed. The Regge is a small river running through the East of the Netherlands and a small part of Germany; it is a subcatchment of the Vecht river catchment. In the summer months, the mean discharge at the outlet to the river Vecht is 7 m^3/s. The catchment area is about 1,000 km^2.The soil type is mainly sandy and the main land use is a mixture of livestock and arable farming, with crops feeding the livestock and the livestock providing manure to the arable operations. Maximum mandatory nutrient levels are exceeded by a factor of two to three.

The model simulations were conducted using NL-CAT (Schoumans *et al.*, 2005). The model consists of four sub-modules: (i) a soil and ground water flow module (SWAP), simulating water discharge to groundwater and surface water; (ii) a soil nutrient cycle and leaching module (ANIMO), describing the organic matter, nitrogen and phosphorus cycle; it focuses on the following processes: nutrient addition, mineralization, volatilization, aeration and (de)nitrification, sorption and phosphate fixation, crop uptake, leaching and overland flow; (iii) a surface water flow module (SWQN) in which the main watercourses are schematized and (iv) a surface water quality module (Nuswalite), indirectly calculating nutrient retention based on dissolved organic and mineral fractions of nitrogen and phosphorus and biomass. The model is mainly based on detailed process descriptions and is pseudo-dynamic in time. The smallest model unit of the soil modules is the plot, defined as a unique combination of land cover, land management, soil, hydrological boundaries and meteorology. The smallest model unit for the surface water modules is the subcatchment. More details about the model can be found in Schoumans *et al.* (2005), together with a description of the set-up and calibration of the model for application in the Vecht catchment. For application in the present study, small changes have been made to this model set-up, which has minor implications for the quality of the calibration (see Bijlsma *et al.*, 2006). To simulate the nutrient build up for 1999, the soil modules were run for the period 1941-1999 and the surface water modules for the period 1990-1999.Uncertainty in the model was introduced from the beginning of this initialization period, setting a different equilibrium for each run. For details of the methods and results of the case study, see Bijlsma *et al.* (2006).

Selection of uncertainty sources for analysis

The uncertainty analysis focused on a few important uncertainty sources of ANIMO. Nevertheless, the model contains other important uncertainty sources. The selection was based on a sensitivity analysis (Groenenberg *et al.*, 1999), analysis of critical parameters and constants (Walvoort *et al.*, in preparation) and expert judgment. The following uncertainty sources were selected:

- fertilizer application load (fertilizer); selected for assessment of a wide range of uncertainty types and assessment of bias;
- phosphorus background concentration of the groundwater (PBC); testing the validity of the selection of uncertainty sources at a small scale for catchment scale use;
- gas diffusion parameters in soil related to aeration and denitrification (denitrification);
- iron and aluminium content of the upper soil (Fe/Al).

Quantitative assessment of selected uncertainties

The selected uncertainties were assessed following a common data-driven approach. For the fertilizer application load, this evidence- based approach was extended by the assessment of a wider range of uncertainty types for which both the existence and the magnitude are uncertain. The assessment of fertilizer application load is described in detail below; for the other selected uncertainties, a summary of the method is given.

The quantitative assessment of fertilizer application covers both manure and artificial fertilizer application and is restricted to the dominant land use of grass and maize cultivation, and the dominant soil type of sand. In the assessment, the following assumptions were made to deal with a lack of data: (i) a fixed relationship between the application of nitrogen and phosphorus: fixed ratios are assumed both for the content of manure and between the application of artificial nitrogen and phosphorus fertilizer; (ii) the relative uncertainty is assumed to be constant over time; the relative uncertainty bandwidth is determined for one year and is then applied to all other simulation years; furthermore, the estimate of the uncertainty for that single year is based on field observations over several years.

Based on data, uncertainty distributions were found showing variability in the field application rate (Table 1). The distributions at the field scale level were upscaled to the plot scale level by the following formula (Refsgaard *et al.*, 2006):

$$\sigma_{\text{plot}} = \sigma_{\text{field}}/\sqrt{N} \tag{1}$$

where σ is the standard deviation and N the number of independent fields in a plot (the number of fields divided by the autocorrelation length of a field). Based on land use maps, the average size of a field is estimated to be 2 ha. The autocorrelation length of a field is assumed to be 1.5 fields for maize and 3 fields for grass; neighboring fields are assumed to

Table 1 Overview of the uncertainty types and associated distributions assessed for fertilizer application (appl.) load on field scale level. STD stands for standard deviation

Uncertainty type	Distribution type	Mean (kg/ha) year 2000	STD (%)	Source and type of data
Bias for appl. nitrogen (N)/phosphorus (P)	Uniform	410 (N) 165 (P)	14	Expert judgment
Effective nitrogen appl.[1] for grass on sand	Normal	287	33	Oenema *et al.* (2002): nitrogen surpluses of 198 fields, 1999
Organic manure nitrogen appl. for maize on sand	Normal	253	44	Fraters *et al.* (2005): non-grassland fields at 60 farms, 1991-1995
Artificial fertilizer nitrogen appl. for maize on sand	Normal	34	91	Reijneveld *et al.* (2000): mean and std. silage maize, 1997. Milk production farms 10000-12000 kg/ha

[1] The reported surpluses for organic manure ($N_{org.man}$), artificial fertilizer (N_{fert}) and grazing cattle manure ($N_{gr.catt}$) have been converted to effective nitrogen surpluses (N_{eff}), by: $N_{eff} = N_{fert} + 0.5N_{org.man} + 0.1 = N_{fert} + 0.5N_{org.man} + 0.1N_{gr.catt}$.

be fed with manure in the same way. The original standard deviation at the field scale is very large, but this variability is expected to average out to a large extent at the catchment scale. More data revealing the presence of uncertainty in fertilizer application loads are not available. However, other sources of uncertainty are expected to exist.

Expert judgment was brought to bear on a search for more uncertainty sources. A bias due to data processing that affects all fertilizer data was identified. Reported measurement data have been processed, based on assumptions about the nutrient contents of manure, animal excretion rates and volatilization rates. For assembling the model input, additional assumptions were made about, for example, manure transport, fertilization trends over time and agricultural management. Since no data are available for these aspects, expert judgment was used to quantify this uncertainty type. A uniform distribution was defined (see Table 1), which has the original model's deterministic application load as its mean. In assessing the minimum of the distribution to be 75% and the maximum to be 125% of the mean, the less biased field application loads served as a reference for the order of magnitude.

To implement the uncertainty analysis, a two-step approach was followed. The bias is for the total amount of fertilizer in the area and thus influences the mean of the uncertainty distribution. A first draw from the uniform distribution represents the total fertilizer application in the catchment. Next, the application load for each plot was sampled from a distribution with this obtained mean and the standard deviation on plot level as calculated by Equation 1.

The results of the uncertainty assessment of the other uncertainty sources are summarized in Table 2. For the assessments, the following assumptions were made (for justification, see Bijlsma *et al.*, 2006): (i) no spatial variation over the catchment (except for the iron and aluminium content of the upper soil); (ii) no temporal variation; (iii) the experimental data used are representative and contain no bias.

The gas diffusion parameters in soil related to aeration and denitrification are the variables p_1 and p_2 (-) in the oxygen diffusion relationship (Bakker *et al.*, 1987):

$$\frac{D}{D_o} = p_1 \varepsilon^{p_2} \tag{2}$$

where D is the oxygen diffusion coefficient in soil relative to the oxygen coefficient D_0 in air ($L^2\ T^{-1}$) and ε is the soil air content (-). The uncertainty in the parameter values were assessed for podzolic, medium textured sandy soils for the subsoil zone. Experimental data for the diffusion relationship were used to assess the parameters p_1 and p_2

Table 2 The median and 90% confidence interval (CI) for the input of each uncertainty source, represented by the median, 0.05 and 0.95 quantile for the total catchment average input. The last column gives the 90% CI as a percentage of the median value

Uncertainty source	Median	0.05-Quantile	0.95-Quantile	% of median
Fertilizer application load	527 kg N/ha (effective N)	442 kg N/ha (effective N)	643 kg N/ha (effective N)	38%
Phosphorus background concentration in groundwater	0.00016 kg/m^3	0.00015 kg/m^3	0.00018 kg/m^3	19%
Gas diffusion parameters in soil	P1: 0.65 P2: 2.46	P1: 0.34 P2: 1.95	P1: 1.59 P2: 2.94	P1: 92% P2: 40%
Iron and aluminium content of the upper soil	56.7 mmol/kg	54.4 mmol/kg	62.4 mmol/kg	14%

simultaneously in a multi-variate analysis. Bootstrapping (Efron and Tibshirani, 1993) was performed to estimate the joint uncertainty distribution of the parameters. For each bootstrap sample, the parameters p_1 and p_2 were estimated by means of non-linear least squares regression.

An uncertainty distribution for the phosphorus background concentration of the groundwater was assessed by aggregating point measurement concentration data. This resulted in a normal distribution representing the catchment's mean phosphorus background concentration.

The uncertainty in the iron and aluminium content of the upper soil (1–120 cm) was assessed by a geostatistical analysis at the plot scale using conditional sequential Gaussian (block) simulation (Goovaerts, 1997). The mean and standard deviation of iron and aluminium concentrations were determined for each soil type and then the variogram was determined. The analysis was conducted for the horizontal spatial variations of iron and aluminium. Vertical segmentation was reflected by the original deterministic ratios.

Assessment of the effects of the selected uncertainty sources on the results

The uncertainty distributions were propagated through the NL-CAT model by means of standard Monte Carlo analysis. The distributions are sampled independently to create 50 realizations; for this number of realizations the mean and standard deviation were sufficiently consistent.

Results and discussion

The results of the case study analysis are used in this section to show that the commonly used practices for uncertainty analysis at large scales are not always valid. In Figure 1, the uncertainty bandwidth for the summer averaged nitrogen and phosphorus concentration for

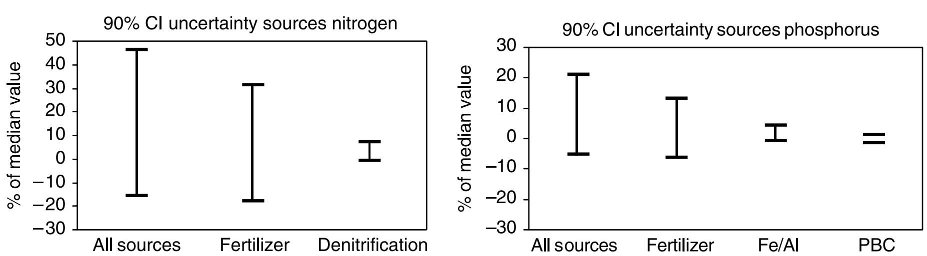

Figure 1 The 90% CI of the uncertainty bandwidth for 1999 at the Regge river outlet for nitrogen (left) and phosphorus (right) as a percentage of the median value, shown together with the contribution of the individual uncertainty sources to the uncertainty bandwidth characterized by the output of the simulation runs with 0.05 and 0.95 quantile input

1999 at the Regge river outlet is shown, together with the contribution of the individual uncertainty sources for nitrogen and phosphorus to this uncertainty bandwidth.

Non applicability of small-scale sensitivity analysis for larger analysis scales

The 'phosphorus background concentration of the groundwater' (PBC) uncertainty source makes a very small contribution to the total uncertainty bandwidth (Figure 1); the 90% confidence interval (90% CI) is just 2.5% of the median value. A larger contribution was expected on the basis of the sensitivity analysis and expert judgement at the plot level. The 90% CI of the plot output loads, averaged over all plots, is 10% of the median value. At the catchment level, this effect disappears. Averaging out effects are not expected, since the input concentration is constant for the complete catchment. Saltelli *et al.* (2000) mention the influence of the model setting on the sources that drive output variations. Conversely, Yoe and Skaggs (1997) note that once the important sources of uncertainty have been identified, this knowledge is relevant for any future study using that model. Either way, in practical applications a sensitivity analysis is usually not performed for every model application at every scale. However, processes in the larger scale model can cause a change in the effects of uncertainty sources compared to the small-scale model.

Restriction to assessment of uncertainty types with a strong evidence base gives conservative estimates

The contribution of the variability in fertilizer application load, as assessed using a data-driven approach, is very small compared to the contribution of the bias (25%) in the application load (Figure 2). For this bias, the existence and magnitude were assessed based on expert judgment. The consulted experts agreed that the uncertainty due to variability alone is much too small to represent the uncertainty in fertilizer application load. Several authors suggest that uncertainty analysis could - and should - be extended to those aspects of scientific enquiry that are beyond empirical testing (e.g. Brown, 2004; Saltelli *et al.*, 2004). The difficulty is that this introduces a large uncertainty about the extent of uncertainty. Assessment of these types of uncertainty by expert judgment is inevitably subjective (Cooke, 1991). However, not assessing such uncertainty types is a subjective choice as well, having a very large impact on the results of the uncertainty analysis as shown by Figure 2, namely a large structural underestimation of the uncertainty bandwidth.

Small biases may easily outweigh variability

Figure 2 also shows the contribution of a bias of only 5% in fertilization application load data in comparison to the variability. The conventional data-driven approach usually focuses on uncertainty due to variability and often fails to explore structural uncertainties such as bias (Brown, 2004). The figure shows that, at large scales, the impacts of a small

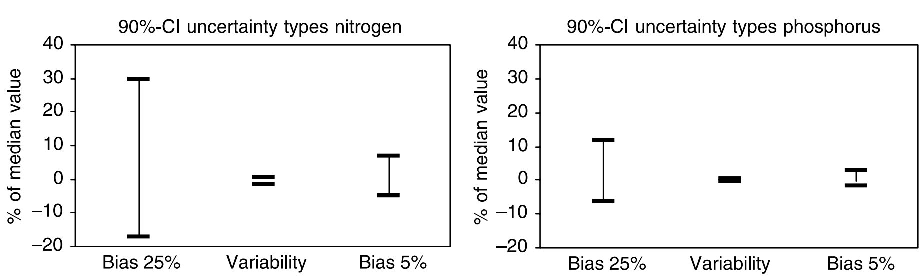

Figure 2 Comparison of the 90%-CI of the variability and the bias as quantitatively assessed for fertilizer application load. Next, the contribution of a bias in the data of 5% is shown

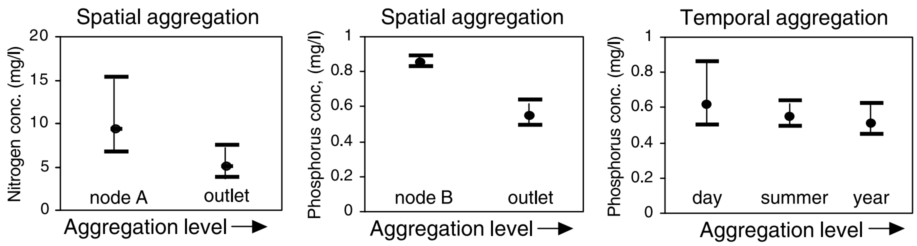

Figure 3 The effects of spatial and temporal aggregation on the nitrogen and/or phosphorus concentration. The nodes are situated halfway the catchment

bias may greatly outweigh the effect of variability. A similar notion can be found in, for example, Oreskes and Belitz (2001) and Brown (2004).

Uncertainty bandwidth may increase for higher aggregation levels

The choice for an output variable with a different spatial or temporal aggregation largely influences the median and uncertainty bandwidth of the results of a study (see Figure 3). When a larger aggregation level of the output variable is chosen, it is generally assumed that the uncertainty bandwidth decreases due to effects of averaging out (e.g. Heuvelink and Pebesma, 1999). However, Figure 3 shows that it can also increase when, for this larger aggregation level, the spatial or temporal variability patterns in the variable concerned become larger.

Conclusions

This paper demonstrates that the following common current approaches and assumptions in uncertainty analysis are not always valid in large-scale uncertainty analysis.

- The most relevant uncertainty sources are often selected - as in our case - based on sensitivity analysis and expert judgment at a small (in our case, plot) scale. These results may differ from the effects at a large (in our case, catchment) scale.
- The assessment of an uncertainty source is usually restricted to the uncertainty types for which clear evidence exists (usually data-driven). Uncertainty types for which the nature and magnitude are highly unknown (uncertain) are left out. This leads systematically to a conservative estimate of the uncertainty bandwidth. Since these uncertainty types can be highly influential, including them gives a more realistic uncertainty estimate. The disadvantage is a less precise and likely subjective uncertainty distribution. However, the choice not to assess these uncertainty types is itself subjective and also very influential.
- The focus of current uncertainty analysis is mostly on data variability. In large-scale analysis, small biases in the data may easily outweigh the effect of large variability; the correlation length scale of biases is mostly much larger than that of variability.
- When a larger aggregation level of the output variable is chosen, the uncertainty bandwidth can decrease due to the effects of averaging out, but it can also increase. This in response to the spatial or temporal variability patterns in the variable concerned.

Our conclusions imply a need for change in current common practice and conceptions in large-scale uncertainty analysis. The first and fourth points do not imply major changes in current practice, but practitioners need to be made aware of the implications of their approach. The second and third points suggest a necessary change in paradigm in which uncertainty analysis becomes an actual reflection of what we are uncertain about and not just a reflection of the uncertainties we understand.

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