Assigning confidence limits to outputs from a nitrate leaching model:

A case study from the River Ure catchment, UK

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Abstract— **Diffuse pollution from agriculture is a major concern for surface water management under the EU Water Framework Directive, and water quality models are frequently used as decision support tools for policy implementation to achieve water quality objectives. The current study uses uncertainty analysis techniques to assign confidence limits to outputs from a nitrate leaching model. A sensitivity analysis determines which input variables require most detailed attention in terms of limiting output error. The issue is illustrated through application of a nitrate leaching model to the River Ure catchment in northern England. Implications for predicting possible outcomes of future, policy-driven, land use change are examined, and recommendations are made regarding the use of such models as decision support tools.**

Keywords: diffuse pollution, nitrates, SLIMMER, uncertainty analysis, Water Framework Directive

I. INTRODUCTION

Diffuse pollution from agriculture is known to be a primary cause of excessive levels of compounds such as nitrates, phosphates and pesticides in water bodies, and implementation of the EU Water Framework Directive (WFD) (CEC, 2000) will require substantial changes in land management practice to achieve the goal of "good ecological status" in all water bodies by 2015. One of the aims of the Catchment Hydrology, Resources, Economics and Management (ChREAM) study (Bateman et al., 2006) at the University of East Anglia, is to assess likely impacts of WFD implementation on agricultural land use, and consequences for water quality and farm incomes. An element of the study has involved analysis of a number of measures, proposed to the Department for Environment, Food and Rural Affairs (Defra) by Cuttle et al. (2007) that could be used to tackle diffuse pollution from agriculture. An example of one such measure is to convert areas of arable land to un-grazed (extensive) grassland.

Water quality modelling is increasingly performed within a GIS framework (Anthony et al., 2009, Grayson et al., 2008, Matthies et al., 2007, Lagacherie et al., 2006), but although development of such models often involves the creation of new input data from existing source data, uncertainty analysis is far from routine and rarely presented with the results. In order for meaningful conclusions to be drawn, information is required as to the accuracy of source data (which is often unavailable) and the associated uncertainty in model output. The current study uses uncertainty analysis techniques to assign confidence limits to outputs from a nitrate leaching model. Model sensitivity to individual input parameters is examined and the findings are discussed in relation to the UK Environment Agency classification scheme for surface water quality.

The case study location was the River Ure catchment in northern England, a sub-catchment of the Humber river basin, the latter being the main focus of the ChREAM study. The Ure catchment covers an area of approximately 91,000 ha, comprising 153 hydrological response units (HRUs) corresponding to areas of land over which surface water drains to discrete river stretches, and encompasses a diverse range of environmental characteristics ranging from grazed uplands with high rainfall in the west, to lowland arable and urban areas with lower rainfall in the east (Fig. 1).

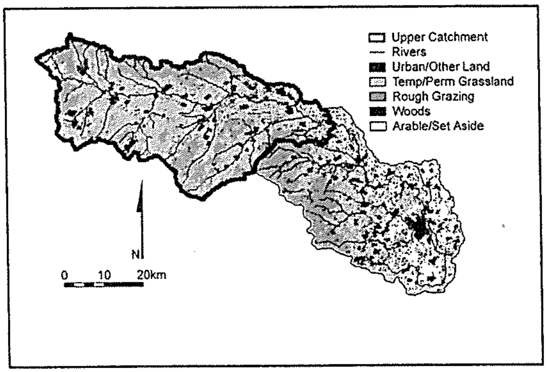

Figure 1. The River Ure catchment.

A nitrate leaching model was used to estimate river nitrate-N concentrations for the period 2000-2003 and these results were evaluated against Environment Agency monitoring data. Uncertainty and sensitivity analysis techniques were then applied to specific model input parameters to obtain a range of possible outcomes for N concentration at catchment and sub-catchment scales.

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II. METHOD

A. *The Nitrate Leaching Model*

The model combines parameters relating to climate, soil type, land use and population density with hydrological data, in a spatially-explicit framework, to derive nitrate-N concentrations at the catchment scale. Land use data were derived from Land Cover Map 2000 (Fuller et al., 2002) and the Defra Agricultural Census for 2004 (http://edina.ac.uk/agcensus), using the method described in Posen et al. (2009); population data were obtained from the Office for National Statistics (2001); soil types were assigned according to the HOST classification system (Boorman et al., 1995); rainfall data were obtained from the UK Meteorological Office Standard Average Annual Rainfall records; evapotranspiration data were taken from the MORECS data set (http://www.metoffice.gov.uk/environment/morecs.html); export coefficients relating to types of agricultural land were defined by the grassland NCYCLE model (Scholefield et al., 1991) and theories from other well-tested models; and crop-specific nitrate available for leaching (NAL) values were obtained from extensive field experimentation data available in the literature. The model set-up is such that nitrate-N (kg/ha) from diffuse sources can be calculated for each HRU according to: the proportional area occupied by each unique land use/soil type combination; NAL values associated with each unique combination (Hutchins et al., 2010); a hydrological transfer function (SLIMMER model: Anthony et al., 1996) driven by information on the field capacity of specific soils and hydrologically effective rainfall for the location. The resulting values are then combined with point source N according to population data and an urban/rural classification system, summed to give annual N values at catchment and sub-catchment scales, and combined with annual river flow (from observed daily data) to derive annual in-river N concentrations at the catchment outlets. In the first instance, the model was run with inputs as described above. This initial model run was taken as the baseline for the uncertainty and sensitivity analyses.

B. *Uncertainty Analysis*

A Monte Carlo simulation was performed using the R programming language (R Development Core Team, 2008) to obtain a range of possible model outcomes for the Ure catchment, so that confidence limits could be assigned to the baseline model outputs. It was considered that climatic inputs, and coefficients relating to the derivation of HER and those used in the SLIMMER function, were tightly constrained; therefore, for the purpose of this study, the values of these parameters were treated as constant. In the case of NAL and field capacity variables, 100 random samples of each were drawn from normal distributions about the mean, with standard deviation values assigned by expert judgement. For each unique land use/soil type combination, the value of its proportional abundance within each HRU was sampled 100 times from each of three normal distributions, within respective 10%, 20% and 30% limits of variability. For each randomly sampled land/soil set, the resulting proportional values were scaled to sum to 1 (i.e. the total available area) for each HRU. Then, using all of the randomly sampled variables, the nitrate leaching model was run 100 times within each of the three different bands of variability for the land/soil proportions. The results were used to assign confidence limits to the baseline model outputs and evaluated against Environment Agency monitoring data and General Quality Assessment (GQA) classes for nitrates in rivers and canals (Table I).

C. *Sensitivity Analysis*

For each of the randomly-sampled parameters in Section II.B, minimum and maximum values were used, in turn, as inputs to the model, to test model sensitivity to each of these variables. In the case of NAL and field capacity, the minimum and maximum input values were taken, respectively, as 2 standard deviations below and above the mean values, and for land/soil proportions, the lower and upper values for each of the three bands stated in Section II.B were used. The effects were assessed in the context of a dry year, a wet year, and as a four-year average over the period 2000-2003.

III. RESULTS

Outputs and confidence intervals for the baseline model are presented in Table II, at sub-catchment and whole catchment scales, the sub-catchment representing approximately the upper (western) half of the Ure catchment (51,000 ha), comprising predominantly temporary and permanent grasslands, and rough grazing areas, with very little arable agriculture (Fig. 1). The modelled results are given in the context of a wet year (2001), a dry year (2003)

TABLE I. UK ENVIRONMENT AGENCY GQA CLASSES

Class	**N Concentration (mg/l)**	**Description**
1	0 - 1.13	Very low
2	1.13 - 2.26	Low
3	2.26 - 4.52	Moderately low
4	4.52 - 6.77	Moderate
5	6.77 - 9.03	High
6	> 9.03	Very high

Source: http://www.environment-agency.gov.uk/

TABLE II. MODELLED AND OBSERVED N CONCENTRATIONS FOR THE RIVER URE

	N Concentrations (mg/l)											
	2001				*2003*				*4 yr mean*			
Catchment extent:	*whole*		*sub-*		*whole*		*sub-*		*whole*		*sub-*	
		*		*		*		*		*		*
Baseline	1.53	2	0.74	1	2.44	3	1.14	2	1.90	2	0.85	1
Std. Dev.	0.63		0.54		1.01		0.83		0.63		0.54	
Minimum	0.90	1	0.20	1	1.43	2	0.31	1	1.27	2	0.32	1
Maximum	2.17	2	1.27	2	3.46	3	1.97	2	2.53	3	1.39	2
Observed	3.03	3	n/a		2.73	3	n/a		2.82	3	n/a	

* Environment Agency GQA Nitrate Clas

and as a four-year average (2000-2003), along with observed N concentrations for the whole catchment. Unfortunately observed data are not available for the upper catchment. Associated Environment Agency GQA classes (Table I) are given for both modelled and observed values.

The most notable results from Table II can be summarised as follows:

- all of the baseline concentrations are lower than observed values for the whole catchment, with only the 'dry year' baseline value falling within the same GQA class as the observed value, but the modelled 'wet year' and 'four-year mean' values falling in the neighbouring, better quality, class;
- highest baseline concentrations occur in the dry year, whereas the highest observed concentration occurs in the wet year;
- modelled values for the upper catchment each occur within a better respective GQA class than those for the whole catchment;
- in terms of GQA classes over a four-year mean, variability in model output ranges from no change in GQA class to a drop in quality by one class, the latter being strongly influenced by high 'dry year' concentrations.

Results of the sensitivity analysis are presented in Table III. These are considered under the same temporal, climatic and catchment subdivisions as the baseline model. Output variability related to each parameter is expressed as percentage variability about the modelled baseline concentrations. The results can be summarised as follows:

- the model exhibits minimal sensitivity to variability in field capacity and, in terms of the effect on GQA class, no change occurs at either sub- or whole catchment level;
- model outputs are most sensitive to variability in NAL, with greater sensitivity occurring at the whole catchment scale than in the upper catchment alone;
- at the whole catchment level, in terms of GQA classes over a four-year mean, output variability with respect to NAL ranges from no change in GQA class to a drop in quality by one class, the latter being strongly influenced by high 'dry year' concentrations;
- model sensitivity to variation in land use/soil proportions increases as the variability boundaries widen: this parameter begins to dominate model output variability when land/soil proportions are allowed to vary by 20% or more;
- at the whole catchment level, in terms of GQA classes over a four-year mean, output variability related to land/soil proportions ranges from no change in GQA class, to a drop in quality by one class for land/soil variability of 20% and above, once again strongly influenced by high 'dry year' concentrations.

IV. DISCUSSION

We are presented with two important issues in the results of the baseline model: (a) all three baseline values are lower than observed concentrations at the catchment outlet, and (b) the baseline model predicts that highest N concentrations will occur in the dry year, whereas observed concentrations are highest in the wet year. One hypothesis for these inconsistencies is that, rather than the mismatch resulting from some element of error in the model or model parameters, the observed values are elevated due to N inputs from another source. It is known that groundwater makes a significant contribution to surface water flow in certain sub-catchments of the Humber basin, and that many groundwater bodies have elevated nitrate levels arising from historic use of agricultural fertilisers. It was thought that groundwater contributions may account for the higher observed than predicted N concentrations in the Ure, and this theory was supported by the differences between modelled and observed values for the wet and dry years. During a wet year, the increased volume of surface water will generally dilute nutrient loadings from agriculture, resulting in lower river concentrations and, conversely, during dry periods, without the diluting effect of a high volume of water, river nutrient concentrations will be elevated. This is seen in the modelled results, but not in the observed data for the Ure, the latter showing the highest N concentration in the wet year and a lower concentration in the dry year. A strong contribution from groundwater with high nitrate levels could account for these observations since, during very wet periods, an elevated water table could increase the supply of nutrients to the river, supplementing those from surface run-off, whereas the nutrient supply from groundwater would be reduced during dry periods, resulting in lower N concentrations. Nevertheless, data suggest that a groundwater nitrate signal is not strong in the Ure (in comparison with some other nearby catchments, e.g. Yorkshire Derwent). There are, however, very high livestock numbers attributable to some HRUs in the Ure. Consequently, the impact of managed manure applications could have been underestimated and could explain underestimation of N concentrations.

TABLE III. SENSITIVITY OF MODELLED N CONCENTRATIONS TO VARIATION IN SPECIFIC INPUT VALUES FOR THE RIVER URE CATCHMENT

Model Parameter	**Percentage Variability about Modelled Baseline N Concentrations**			
	catchment extent	*2001*	*2003*	*4 yr mean*
Field Capacity	whole	0.0	1.8	1.0
	sub-	0.0	0.3	0.1
NAL	whole	25.3	25.1	25.2
	sub-	19.5	18.4	19.4
Land/Soil Proportion - 10% bounds	whole	13.4	16.3	13.4
	sub-	13.5	13.5	13.5
Land/Soil Proportion - 20% bounds	whole	26.8	26.8	26.8
	sub-	27.2	38.3	27.1
Land/Soil Proportion - 30% bounds	whole	40.2	40.1	40.2
	sub-	40.6	40.7	40.7

Due to these discrepancies, only the modelled value for the dry year is high enough to fall within the same GQA nitrate class as the observed data (i.e. Class 3, moderately low) – this is the class within which all of the observed data fall. Modelled values for the wet year and the four-year mean fall within Class 2 (low), but at the upper confidence limit for the four-year mean, values correspond to GQA Class 3. No observation data are available for the upper catchment, but the consistently lower values of modelled N concentration for this sub-catchment, compared with the whole catchment, correspond to land use differences – i.e. predominantly agricultural grasslands and rough grazing in the upper catchment, with most arable crops (and attendant higher NAL values) occurring in the lower catchment.

In terms of model sensitivity, variations in field capacity have little impact, but changes both in NAL values and in land use/soil proportions have a much greater influence on model output. Expressed as percentage variability about the baseline value (Table III), model outputs are most sensitive to changes in NAL (assuming baseline values for land/soil inputs). However, when NAL inputs are held constant, the greatest influence on model output arises when land/soil proportions cross the 20% boundary in variability. This, combined with the suggestion that deterioration in quality is most likely to occur in unfavourable combinations of land use and low rainfall, has important implications for possible policy- or climate-driven land use change. For example, policy measures which promote conversion of arable land to extensive grassland are likely to be highly beneficial in terms of improving water quality if careful spatial targeting is used in their implementation. Conversely, a rise in temperature which allows the extension of certain types of agriculture into previously unsuitable areas may have a detrimental effect on water quality, particularly if accompanied by lower rainfall and high NAL values. As this study has suggested, the situation could be further complicated by groundwater contribution to surface water flow in some river catchments.

V. CONCLUSIONS AND RECOMMENDATIONS

This work highlights some important issues surrounding the use of water quality models as decision support tools for surface water management. Uncertainty analysis techniques reveal that the model underestimates N concentrations at the River Ure catchment outlet, even at the upper extreme of output confidence limits. This discrepancy may be due to contributions from sources such as groundwater nitrate or livestock manure in the observed data, emphasising the importance of including monitoring data and accounting for site-specific conditions in the modelling process. Further model testing is proposed on other river catchments, which may help to clarify some of the issues encountered in this analysis and provide useful insights into how the model could be improved. The sensitivity analysis suggests that close attention should be paid to the accuracy of NAL input values, as variations in these have a large influence on model outputs. Additionally, sensitivity of the model to large variations in land use/soil combinations may have important implications for land management options. In this respect, it is felt that the availability of agricultural census data at a finer resolution could reduce uncertainties from this source. The study indicates that careful consideration should be given to the spatial targeting of land use policy measures, with particular emphasis on limiting the potential for deterioration of water quality under climate change.

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