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Spatially distributed modelling in support of the 2013 review of the Nitrates Directive

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Executive Summary

Background to research

The Nitrates Directive (91/676/EEC) requires EU member states to monitor nitrate concentrations and to designate those areas considered to be at risk as Nitrate Vulnerable Zones (NVZs). Designations are reviewed every four years, using a methodology proposed by the Scottish Environmental Protection Agency (SEPA) and approved by the Scottish Government. This document describes the spatially distributed modelling undertaken by the James Hutton Institute at the request of the Scottish Government. It is one of the strands of evidence incorporated into the 2013 Nitrates Directive review.

Objectives of research

Objective 1

To use a physically-based, dynamic modelling approach to estimate losses of nitrate from the land to Scotland's surface and groundwaters.

Objective 2

To demonstrate that the model is capable of adequately simulating nitrate leaching and to use it to estimate nitrate concentrations in the groundwater bodies defined under the Water Framework Directive.

Objective 3

To produce maps and summaries of the model output that can be used as one strand of evidence in the 2013 Nitrates Directive review.

Key findings and recommendations

Objective 1

- The Nitrogen Risk Assessment Model for Scotland (version 2; NIRAMS II) has been used to model nitrate concentrations at national scale for the period from 2006 to 2010. The model was calibrated against surface water data and used to investigate nitrate concentrations in waters draining from the soil zone to the groundwater.

Objective 2

- Model output has been summarised for each of the 300 groundwater bodies defined by the Water Framework Directive.
- In most regions not associated with impermeable clays or denitrifying geology, the model's predictions are in close agreement with observed data. It is therefore reasonable to use the model as one of the strands of evidence incorporated into the 2013 Nitrates Directive review.
- The model significantly over-predicts nitrate concentrations for six of the 42 groundwater bodies with robust monitoring data. However, these six bodies are all associated with low permeability clay layers or deep unsaturated zones, both of which inhibit the movement of pollutants from the surface to the groundwater. Some of them also have iron- and sulphur-rich bedrock geology, which leads to high rates of denitrification from within the groundwater itself. The model does not attempt to account for processes taking place below the soil zone, so there are sound physical explanations for the model's poor performance in these areas.
- Different model parameterisations produce different quantitative results, but the output is consistent when translated onto a categorical scale appropriate for the 2013 review. The results are therefore considered to be robust against uncertainties introduced by the model's parameterisation.

Objective 3

- Maps showing the modelled average nitrate concentration in each groundwater body have been produced for a variety of different model parameterisations. These can be used in conjunction with other lines of evidence to assess the risks to water quality from diffuse nitrate pollution.
- The model predicts high nitrate concentrations for a number of groundwater bodies located around the inner Firth of Forth that are not currently within the NVZ boundaries. However, in most of these cases the confidence in the model output is low, due to the presence of clay layers and denitrifying lithologies.
- In some areas where the model is expected to perform well, there are predictions of high nitrate concentrations in groundwater bodies that are located outside of the exiting NVZ boundaries. Conversely, some bodies within the existing boundaries are associated with low modelled concentrations. These groundwater bodies warrant more detailed consideration during the 2013 review, incorporating other strands of evidence to evaluate the overall risk to water quality.

Key words

Nitrates Directive, Nitrate Vulnerable Zone, modelling, NIRAMS II, diffuse nitrate pollution, land use, groundwater

Abbreviations

BGS	British Geological Survey
DEFRA	Department for Environment, Food and Rural Affairs
EMEP	European Monitoring and Evaluation Programme
FAO	Food and Agriculture Organisation of the United Nations
GWB	Groundwater body
HOST	Hydrology of Soil Types
IACS	Integrated Administration and Control System
JAC	June Agricultural Census
MCMC	Markov Chain Monte Carlo
NIRAMS II	Nitrogen Risk Assessment Model for Scotland (version 2)
NVZ	Nitrate Vulnerable Zone
RMSE	Root Mean Squared Error
SEPA	Scottish Environmental Protection Agency
WFD	Water Framework Directive

A note on units

All nitrate concentrations in this report are given as milligrams per litre of the nitrate ion (NO_3^-), not milligrams per litre of nitrate-N, as is often used in the academic literature. In the units adopted here, the maximum allowable concentration of nitrate in drinking water (as set out by the Drinking Water Directive) is 50 mg/l. In other publications, this limit may be written as 11.3 mg/l of nitrate-N.

To convert from mg/l of nitrate to mg/l of nitrate-N, divide by 4.43.

1.0 Introduction and objectives

The Nitrates Directive (91/676/EEC) requires EU member states to identify areas where nitrate concentrations in surface and groundwaters either exceed or are likely to exceed 50 mg/l. Such areas must be designated as Nitrate Vulnerable Zones (NVZs), and within these programmes of measures must be implemented with the objective of reducing nitrate contamination.

Under the rules of the Directive, designations must be reviewed every four years. For the 2013 review, the Scottish Environmental Protection Agency (SEPA) was asked to develop a new classification methodology in consultation with the Scottish Government, Scottish Natural Heritage and the National Farmers' Union of Scotland. Their proposed approach aims to incorporate a broader range of evidence than previous assessments, as well as being more consistent with other key legislation such as the EU Water Framework Directive (WFD).

This document describes the spatially distributed modelling undertaken by the James Hutton Institute at the request of the Scottish Government. It is one of the strands of evidence incorporated into the 2013 review. The objectives were as follows:

- **Objective 1**: To use a physically-based, dynamic modelling approach to estimate losses of nitrate from the land to Scotland's surface and groundwaters.
- **Objective 2**: To demonstrate that the model is capable of adequately simulating nitrate leaching and to use it to estimate nitrate concentrations in the groundwater bodies defined under the Water Framework Directive.
- **Objective 3**: To produce maps and summaries of the model output that can be used as one strand of evidence in the 2013 Nitrates Directive review.

2.0 Project background and key datasets

2.1 Existing Nitrate Vulnerable Zones

Four areas of Scotland are currently designated as NVZs (Fig. 1):
- Lower Nithsdale,
- Lothian and Borders,
- Strathmore and Fife,
- Moray, Aberdeenshire, Banff and Buchan.

These regions were first identified in 2002 and last reviewed in 2009 (Scottish Government, 2009). The aim of the current review is to establish whether these boundaries are still appropriate, given the most recent monitoring data and the new classification methodology.

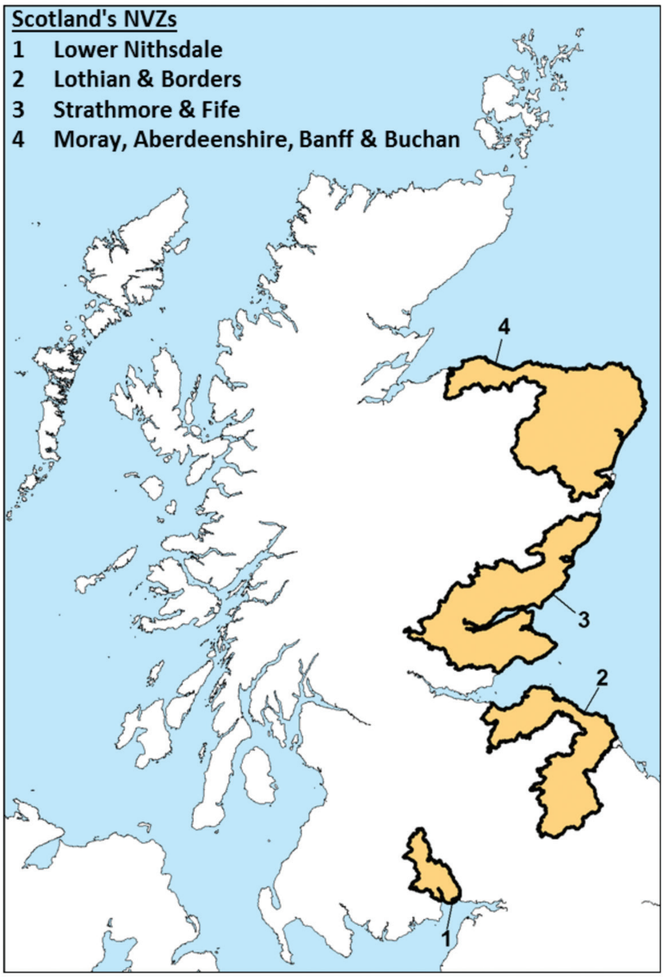

Fig. 1: The geographic extent of Scotland's four NVZs, as defined in 2002.

2.2 Groundwater bodies

Historically, NVZ designations in Scotland have been based primarily on groundwater nitrate, as previous work showed that contaminated surface waters only occurred in areas where groundwater concentrations were also high (Scottish Government, 2009). In contrast to previous review cycles, the 2013 review makes use of the groundwater bodies (GWBs) defined as part of the WFD. These divide Scotland into approximately 300 sub-areas based on the intersection of key geological boundaries with surface water catchments (Fig. 2).

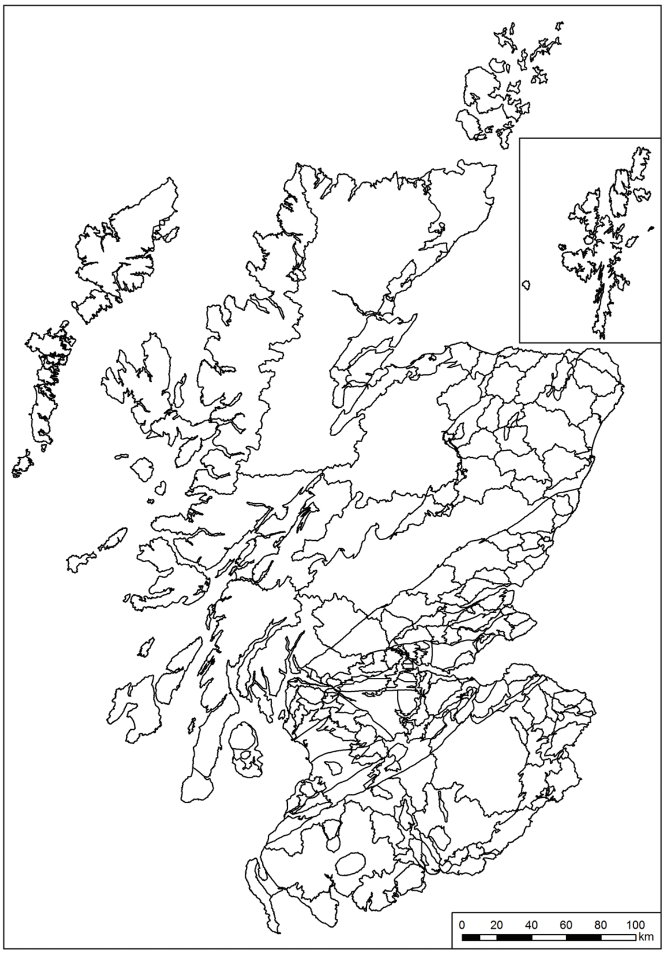

Fig. 2: WFD groundwater bodies. Based on data supplied by SEPA and the British Geological Survey (BGS).

The risk posed to water quality by diffuse nitrate pollution in each GWB has been assessed using a methodology set out in Annex 3 of the Nitrate Vulnerable Zone Review (SEPA, 2013). For modelling purposes, it is assumed that there is a close connection between most surface waters and groundwaters in Scotland, and that nitrates in both are derived from the same source. It is further assumed that groundwater bodies represent areas of similar land use and similar pathway susceptibility to nitrate contamination. For these reasons, similar nitrate concentrations would, in general, be expected across each body. In other words, the GWBs define areas over which groundwater observations and model predictions may be averaged.

2.3 Observed data

As well as maintaining a nationwide network of surface water monitoring sites, SEPA also monitors groundwater nitrate concentrations in over 300 boreholes across the country. Fig. 3 shows the average nitrate concentration measured at each of these locations over the period from 2006 to 2011. The colour scheme used is based on thresholds identified by the WFD: average nitrate concentrations in excess of 37.5 mg/l are usually taken to indicate "poor status", whereas values between 28.0 and 37.5 mg/l indicate "good status", but with a significant risk of deterioration.

There are a number of difficulties in using the observed groundwater data to characterise nitrate concentrations at the GWB scale. In particular, the groundwater monitoring network is relatively sparse (approximately one borehole per 100 km^2 in agricultural areas). This is due to the limited availability of pre-existing boreholes (e.g. for abstraction) and the high costs and logistical challenges associated with constructing purpose-drilled sites. In addition, the highly variable fracture-flow typical of many Scottish aquifers means that sample data from abstractions with small yields, or from purpose-drilled monitoring boreholes, are especially susceptible to local influences, such as contamination from septic tank soakaways or poor manure storage. Further details regarding the existing monitoring network can be found in section 3 of the Nitrate Vulnerable Zone Review (SEPA, 2013).

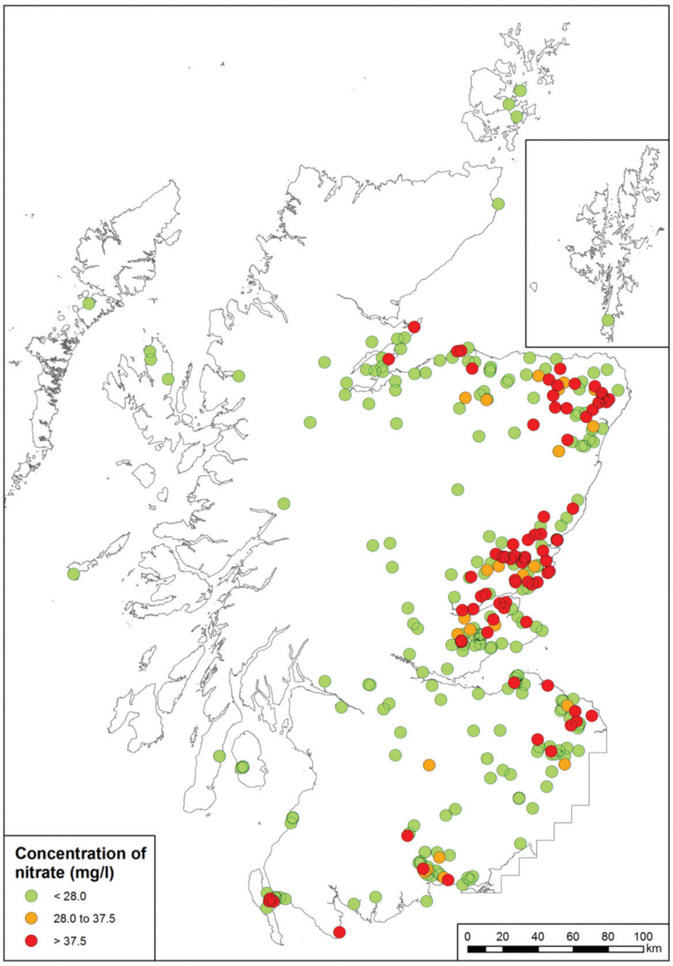

Fig. 3: Average groundwater nitrate concentrations (2006 to 2011) as measured at SEPA boreholes.

3.0 Modelling of nitrate concentrations

3.1 Rationale for modelling

In order to understand the risks posed to Scottish groundwaters by diffuse nitrate pollution, it was necessary to estimate average nitrate concentrations within each GWB. However, due to the limited observed data in some locations, a degree of spatial interpolation was required. Statistical interpolation techniques (e.g. kriging) have difficulty accommodating certain features of the groundwater data, such as the "hard" boundaries between GWBs. In addition, diffuse nitrate pollution is known to be closely associated with land use and agricultural intensity (e.g. Hooda et al., 1997; Weatherhead & Howden, 2009) and it is therefore useful to incorporate this information in as much detail as practicable.

Previous studies have developed and applied mathematical models to assess nitrate losses to water bodies (e.g. Dunn et al., 2004 a and b). This study has adopted a similar spatially distributed, dynamic modelling approach, in which land use and agricultural information were combined with meteorological data to produce gridded estimates of nitrate concentrations. Once calibrated and tested against observed datasets, the model could be used to estimate nitrate losses to groundwater from the bottom of the soil profile. This gives an indication of the potential impact of agricultural activities on groundwater nitrate concentrations, which in turn can be used to assess the vulnerability of each GWB to diffuse nitrate pollution.

3.2 Model structure and input data

Modelling was undertaken using the Nitrogen Risk Assessment Model for Scotland (version 2; NIRAMS II), which is a development of the original NIRAMS model of Dunn et al. (2004 a and b). The model is spatially distributed with a 1 km by 1km grid resolution and is best considered in two parts – a water balance module and a nitrate leaching module (Fig. 5). The water balance module incorporates information representing climate, soil properties and land use patterns in order to predict runoff, which is then passed to the nitrate leaching module. This combines the water balance results with detailed information representing agricultural activities to estimate the amount of nitrate leaching from the soil at each time step. The model considers three possible flow pathways for the leached nitrate: overland flow, shallow sub-surface flow and deeper groundwater flow (Fig. 5). The key outputs are 1 km^2 resolution grids representing the amount of water and nitrate following each pathway at each time step. These grids can be aggregated both spatially and temporally to give estimates of the total runoff and amount of nitrate leached within particular areas and time periods.

NIRAMS II makes use of the following input datasets:

- Climate grids from the UK Met Office, with potential evapotranspiration estimated using the FAO56 modified Penman-Monteith methodology (Allen et al., 1998)
- Soil properties from the Hydrology of Soil Types (HOST) database (Boorman et al., 1995)
- Land use data from the Integrated Administration and Control System (IACS)
- Livestock numbers from the June Agricultural Census (JAC)
- Atmospheric deposition estimates from the European Monitoring and Evaluation Programme (EMEP)

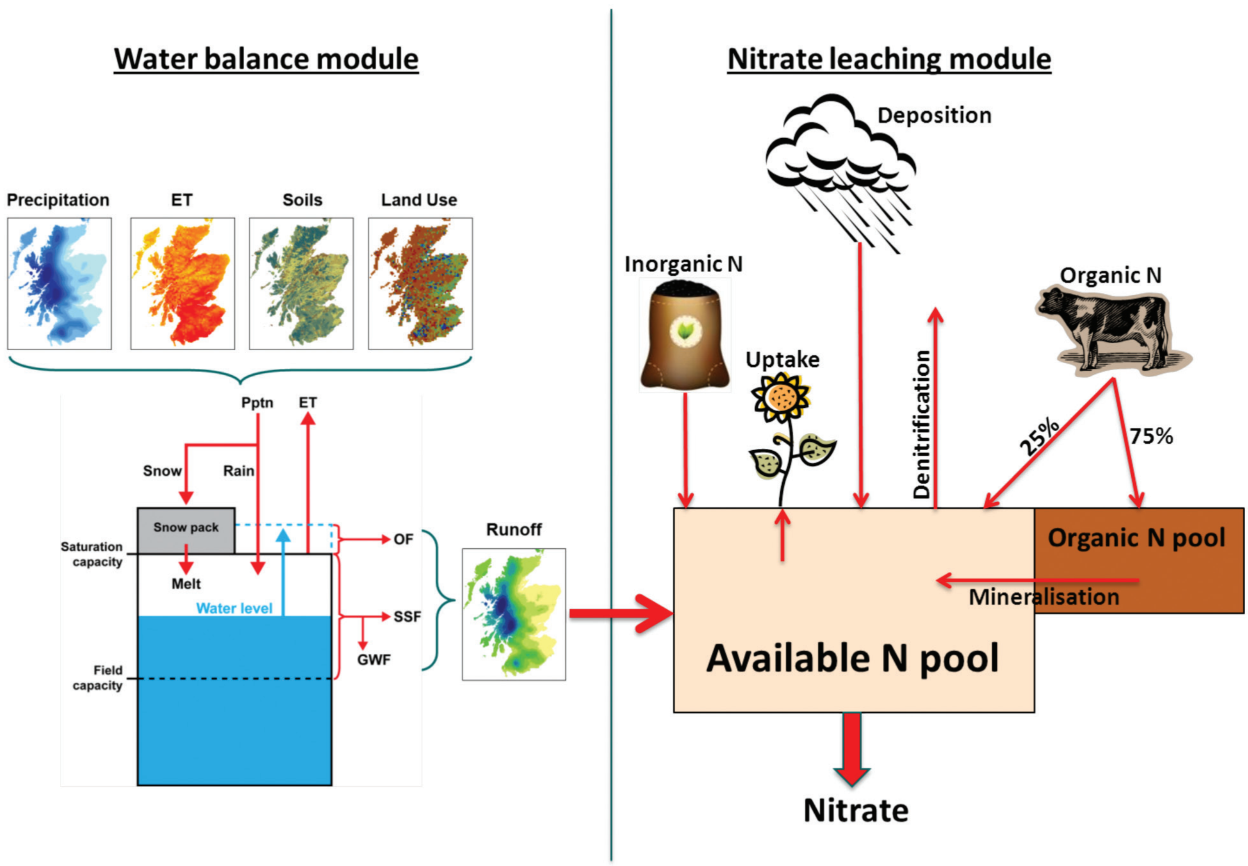

Fig. 5: Illustration of the NIRAMS II model structure, showing key input datasets and physical processes. OF, overland flow; SSF, shallow sub-surface flow; GWF, groundwater flow.

3.2.1 Pre-processing of land use information

In order to make information from the agricultural census compatible with the model's structure, some pre-processing of the data was required. The IACS data is collected annually by the Scottish Government and provides detailed information on the crops grown in the majority of agricultural fields across Scotland. Gaps in the datasets from 2001 to 2010 inclusive were first patched using information from the Land Cover Map 2007 (Morton et al., 2011), and then combined with the results of the British Survey of Fertiliser Practice (DEFRA, 2012) to obtain estimates for the application rate of inorganic nitrogen fertiliser in each field. These results were aggregated to 1 km resolution using area-weighted averaging to produce gridded estimates of the amount of inorganic nitrogen applied to each grid cell in each year.

The JAC data are also collected annually and provide information on the number, age and type of livestock owned by each business receiving agricultural subsidies. The amount of organic nitrogen excreted annually by each animal class was taken from manure planning documentation issued to farmers within NVZs (Scottish Government, 2008), and these figures were used to estimate the total amount of organic nitrogen produced each year by each business. This was then distributed spatially over appropriate land classes at the business scale, using a rule set designed to be broadly compatible with the application limits currently in force within the NVZs. This information was also aggregated to 1 km resolution to create a gridded time series of organic nitrogen application. The annual estimates of the amount of organic and inorganic nitrogen applied were distributed temporally using a set of idealised time series that define, for a variety of crop classes, the length of the growing season, the amount of nitrogen uptake and the timing of fertiliser application. This process made it possible to incorporate the extremely detailed crop and livestock information from the agricultural census into a nitrogen balance with the same spatial and temporal resolution as the key datasets underpinning the water balance module.

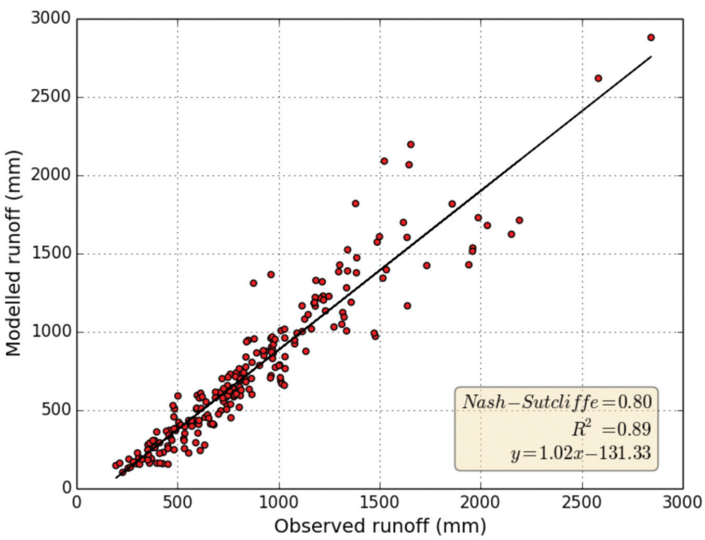

Fig. 6: Modelled versus observed annual runoff at the 56 HMS sites for the years 2001 to 2006 inclusive.

3.3 Calibration and testing

NIRAMS II is not a groundwater model, in the sense that it does not contain any physical representations of groundwater mixing or aquifer systems. Instead, the model simulates the concentration of nitrate draining to the groundwater from the bottom of the soil profile. It is therefore not appropriate to calibrate the model directly to borehole data, although over long time periods groundwater nitrate concentrations might be expected to reflect those in the incoming waters.

By combining the water following the overland, shallow sub-surface and groundwater flow pathways, it is possible to use the model to simulate average surface water nitrate concentrations at annual timescales. The model was therefore first calibrated and tested against surface water data, and the most promising parameter sets were then compared to the groundwater data to investigate the extent to which groundwater concentrations reflect nitrate inputs from the surface.

3.3.1 Water balance component

The water balance module (Fig. 5) was used to estimate annual runoff for the years 2001 to 2006 inclusive for each of the catchments in the Harmonised Monitoring Scheme (HMS; Simpson, 1980). This network provides one of Scotland's best long-term water quality datasets, comprising 56 medium to large catchments spread across the Scottish mainland. Fig. 6 shows the annual model predictions for runoff compared to the observed data.

The model performs acceptably, with Nash-Sutcliffe and R^2 values greater than or equal to 0.8 and a best-fit line with a slope that is very close to one. However, it is clear that the model consistently underestimates runoff by, on average, about 130 mm/yr. This discrepancy could be caused by a number of factors, such as the spatially interpolated Met Office precipitation datasets consistently underestimating rainfall, or the stage-discharge equations at the HMS sites overestimating river flows. Other possible sources of error are the estimates of potential evapotranspiration obtained using the FAO56 Penman-Monteith method (Allen et al., 1998), which ideally requires gridded estimates of both maximum and minimum relative humidity, whereas in practice only mean relative humidity grids are available. Although it is still possible to perform the calculations using these data, the results are known to be less reliable. With this in mind, the scale of error within the water balance simulations seems to be within the bounds of measurement error in the input datasets.

3.3.2 Surface water nitrate

The model was used to simulate surface water nitrate concentrations for each of the 56 HMS catchments for the years 2001 to 2006 inclusive. Although the nitrate leaching module of NIRAMS II has been designed to be as simple as possible, there are a number of poorly constrained model parameters that can be adjusted (calibrated) in order to match observed leaching rates. A common feature of the calibration process is presence of "equifinality" (Beven and Freer, 2001), where multiple different parameter sets give an equally good fit to the observed data. This is particularly an issue in complex models that can have 10s or 100s of parameters. However, even for a minimal parameter model such as NIRAMS II, it is rarely possible to choose a single parameter set for any given modelling application. Instead, a wide variety of initial parameter sets are considered, and all of those meeting basic "goodness-of-fit" criteria are accepted as candidate parameterisations. The remainder of the modelling is then performed using a representative sample of the candidate pool, thereby giving an indication of the uncertainty encapsulated by the model's parameterisation.

The nitrate leaching module of NIRAMS II has four main calibrating parameters, all of which are dimensionless. These are shown in Table 1, together with physically plausible minimum and maximum values defining the ranges over which they could reasonably be varied.

Parameter name	Parameter description	Minimum	Maximum
Organic nitrogen factor	Proportion of nitrogen in organic manure that becomes immediately available for leaching	0.1	0.6
Mineralisation factor	Coefficient influencing the rate of mineralisation	0.1	0.5
Denitrification factor	Coefficient influencing the rate of denitrification	0.01	0.05
Leaching exponent	Exponent influencing the rate of leaching	0.5	1.5

Table 1: Key calibration parameters for the nitrate leaching module of NIRAMS II.

A variety of methods exist for effectively sampling model parameter spaces, many of which make use of Markov Chain Monte Carlo (MCMC) algorithms. However, these approaches typically involve running many thousands of simulations, which can quickly become intractable if the model itself is computationally intensive. Although the four-dimensional parameter space associated with the nitrate leaching module is small compared to most alternative models, the spatially distributed nature of NIRAMS II means that individual run times are comparatively large. As a result, it was not possible to run more than a few hundred simulations in the time available for the 2013 review. For this reason, a semi-automated calibration procedure was adopted, whereby the model was initially run using parameter sets distributed uniformly across the parameter space. Diagnostic plots and summary statistics for each run were tabulated and these were then assessed manually to identify promising regions of the parameter space for further investigation. This process was repeated iteratively to constrain promising parameter combinations.

Model calibration began with two initial parameter searches involving 27 and 64 model runs respectively. Promising areas of the parameter space were then further explored by two more searches involving 81 runs each. For each of the 253 model runs, predictions of the average annual surface water nitrate concentration (in each of the 56 HMS catchments for the years 2001 to 2006) were compared to observed values. Goodness-of-fit for each run was assessed by visually inspecting scatterplots, tabulating Nash-Sutcliffe, R^2 and root mean squared error (RMSE) values, and by evaluating the slope and intercept of the best-fit line. At the end of this process, four candidate parameter sets were considered to give superior results compared to the others (Table 2). Although different, these parameterisations are all located in the same part of the parameter space, suggesting that the likelihood surface has just a single (potentially broad) peak on which the best parameter combinations are distributed. This implies that equifinality is unlikely to be a major concern in this instance, although it is still useful to consider the uncertainty in the model output represented by the four alternative parameterisations.

Modelled versus observed annual concentrations for two out of the four candidate parameter sets are shown in Fig. 7.

Run (of 81)	Calibration parameters				Goodness-of-fit statistics				
	Organic N factor	Mineralisation factor	Denitrification factor	Leaching exponent	Nash-Sutcliffe	R^2	RMSE	Slope	Intercept
1	0.2	0.15	0.01	1	0.68	0.79	0.98	1.03	1.09
6	0.2	0.15	0.02	1.2	0.69	0.75	0.99	0.96	1.09
32	0.25	0.15	0.02	1.1	0.72	0.75	0.94	0.91	1.22
59	0.3	0.15	0.02	1.1	0.70	0.75	0.97	0.93	1.37

Table 2: Candidate parameter sets identified during calibration of NIRAMS II to surface water data

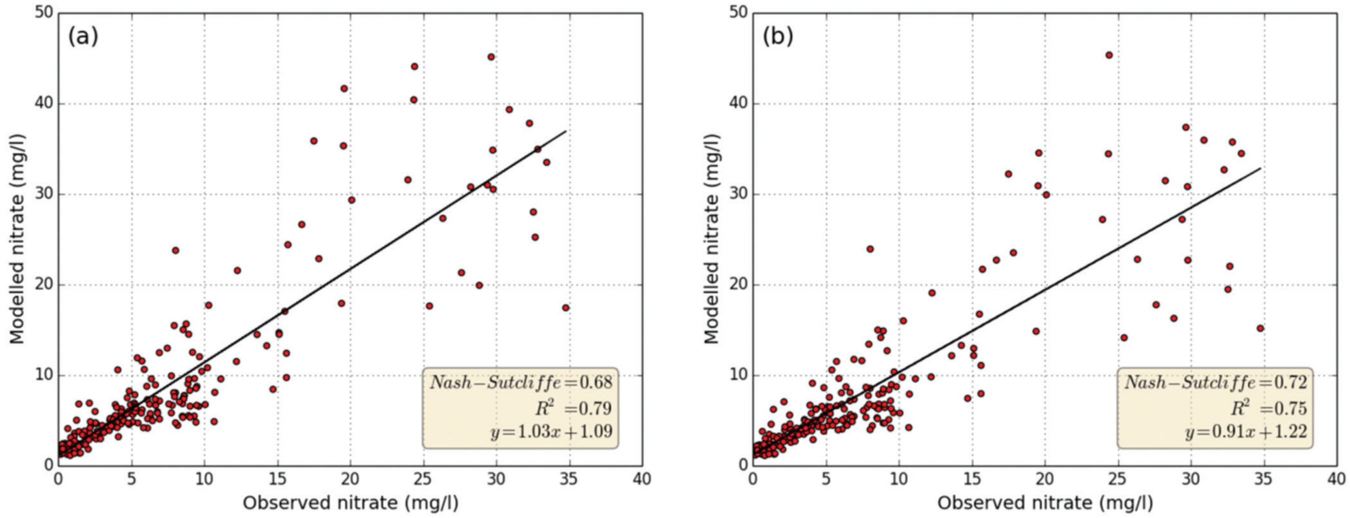

Fig. 7: Modelled versus observed annual surface water nitrate concentrations for two of the candidate parameter sets. (a) Run 1; (b) Run 32 (see Table 2).

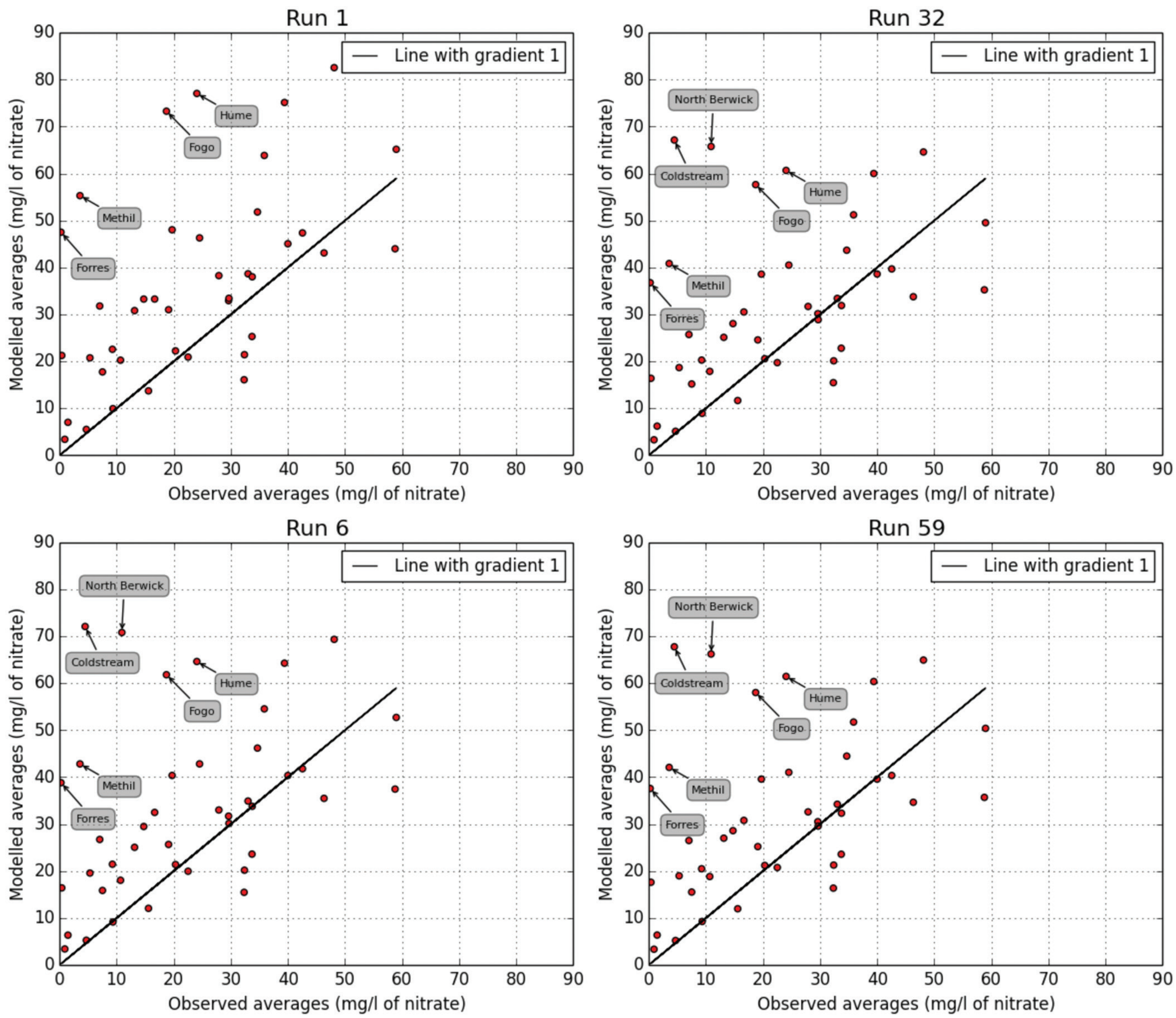

Fig. 8: Observed groundwater nitrate concentrations (averaged by GWB) compared to the modelled average concentrations in water following the groundwater flow pathway. One plot is shown for each of the four candidate parameter sets (Table 2) and major outliers are labelled. Observed averages are for the period from 2006 to 2011; modelled averages are from 2006 to 2010.

3.3.3 Groundwater nitrate

Although NIRAMS II does not directly simulate groundwater nitrate concentrations, it is insightful to compare the modelled concentrations of water following the groundwater flow pathway (Fig. 5) with the observed borehole data. Because of the possibility of local contamination, it is not appropriate to compare the model output to data from individual boreholes. Instead, the observed data were first aggregated to GWB level by calculating the average concentration of all the boreholes within each GWB for the period from 2006 to 2011. In order to ensure that the observed averages were reasonably robust, any GWB with fewer than three boreholes was removed from consideration, leaving 42 GWBs for comparison with the modelled data. Fig. 8 shows the modelled versus observed averages for the four candidate parameter sets.

For aquifer systems with very large volumes or long residence times, there is no reason to expect a simple relationship between the average concentration of nitrate inputs over 5 years and the measured concentrations at boreholes. Nevertheless, the plots in Fig. 8 generally show clear positive relationships, suggesting that in most cases groundwater nitrate concentrations over five year time scales are closely related to the average concentration of inputs from the surface.

All of the plots in Fig. 8 also show a number of distinct outliers: regardless of the parameterisation chosen, the model always over-predicts concentrations in the Forres, Methil, Fogo, Hume, Coldstream and North Berwick GWBs. These represent 14% of the total number of GWBs where modelling and monitoring were compared. (Note that for "run 1", the Coldstream and North Berwick outliers are located beyond the margins of the plot).

The outliers labelled on Fig. 8 are interesting because they refer to GWBs that are known to have substantial clay cover or deep unsaturated zones, both of which restrict the connectivity between surface and groundwaters in these locations. In the North Berwick GWB, for example, a study of the West Peffer Burn catchment by SEPA (2007) identified pesticide contamination in surface waters but not in the groundwater, indicating that there is only limited transfer of pollutants from the soil zone to the aquifer. In addition, the Coldstream, Fogo and Hume GWBs are all associated with iron- and sulphur-rich Carboniferous rocks, which lead to enhanced natural denitrification. With these considerations in mind, the observed concentrations for these GWBs are expected to be lower than the modelled values, since the model does not account for processes taking place beneath the soil zone, nor does it make allowance for the "protecting" effect of low permeability clays.

For the other GWBs, the model performs reasonably well: simple linear regression with the six labelled outliers removed gives R^2 values of around 0.6, regardless of the model parameterisation chosen. This suggests that in areas with good connectivity between the surface and the groundwater, the average concentration of water leaching from the soil profile over a 5 year time scale is one of the key factors influencing groundwater nitrate concentrations.

Of the four possible model parameterisations shown in Fig. 8, three compare favourably to the groundwater data, but the fourth, "run 1", significantly over-predicts concentrations in the vast majority of GWBs. It was therefore eliminated from further consideration, and runs 6, 32 and 59 were used to estimate agricultural losses of nitrate to the groundwater.

3.4 Model output and discussion

The three candidate parameter sets (runs 6, 32 and 59) were used to generate 1 km resolution grids representing the total groundwater flow and amount of nitrate leached from each grid cell during the years from 2006 to 2010 inclusive. The cell values within each GWB were then summed to give estimates of the total groundwater drainage and nitrate load. From these totals it was possible to calculate, for each GWB, the average modelled nitrate concentration draining to the groundwater over this five year period.

Fig. 9 shows the existing NVZ boundaries together with the GWBs, coloured according to the modelled average nitrate concentrations from run 32. Fig. 10 shows two more versions of the same map, but using model output from parameter sets 6 and 59. The colour scheme used on these maps corresponds to relevant legislative thresholds: 50 mg/l represents the maximum allowable concentration in drinking water under the Drinking Water Directive; 37.5 and 28 mg/l are the thresholds defined by the WFD for "poor status" and "at risk" respectively. Concentrations of less than 28 mg/l are generally considered to represent low risk, except in areas that are deemed to be particularly sensitive, such as the Montrose Basin and the Ythan estuary.

Although the three model parameterisations produce different results, once the quantitative predictions have been translated into risk categories the differences become minor; the three parameter sets give essentially the same overall picture of water quality risk across Scotland. This suggests that the model output is reasonably robust against the uncertainty introduced by the model's parameterisation.

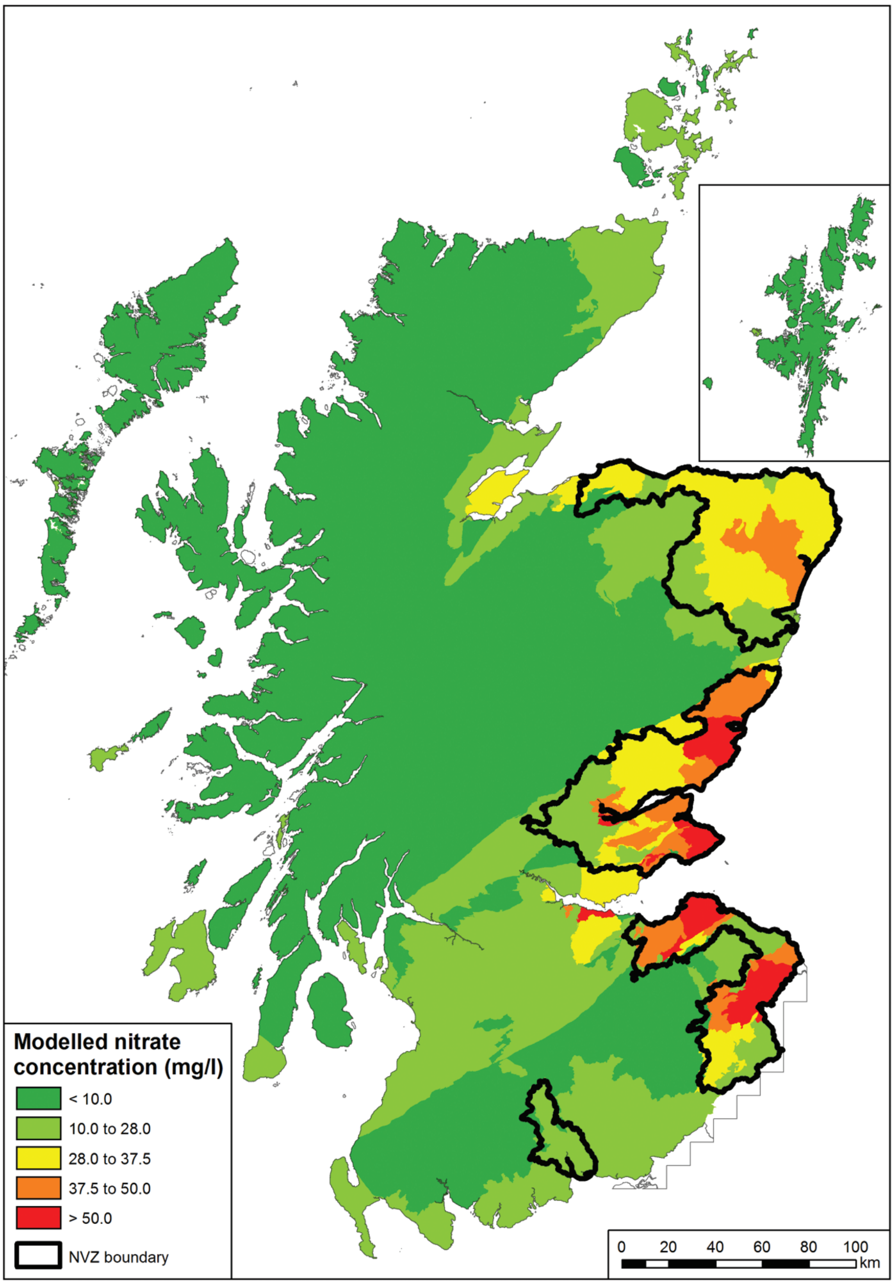

Fig. 9: Modelled nitrate concentrations for each GWB for the "run 32" parameter set (Table 2). Values shown are averages for the period from 2006 to 2010.

On the whole, the GWBs identified as being at high risk from nitrate pollution are situated within existing NVZ boundaries. The main exceptions to this are those located either side of the inner Firth of Forth, such as Livingston, Burntisland and particularly South Queensferry and Kinneil, all of which are underlain by Carboniferous bedrock and might therefore be expected to have high denitrification rates (see section 3.3.3). Because of this, it is likely that the model is over-predicting nitrate concentrations in these areas, so the output must be interpreted with caution.

Elsewhere, the model predicts reasonably high concentrations for the Finavon GWB, just beyond the present north-western margin of the Strathmore and Fife NVZ, and also in the Black Isle GWB, to the west of the Moray, Aberdeenshire, Banff and Buchan NVZ (Fig. 1). The geology in these two areas is not likely to be associated with high rates of denitrification, nor are there extensive clay layers to limit the interaction between surface and groundwaters. The model therefore suggests that these regions should be examined more closely using other strands of evidence. Conversely, within the existing NVZ boundaries there are a number of GWBs with low modelled nitrate concentrations, which may also warrant detailed consideration during the review.

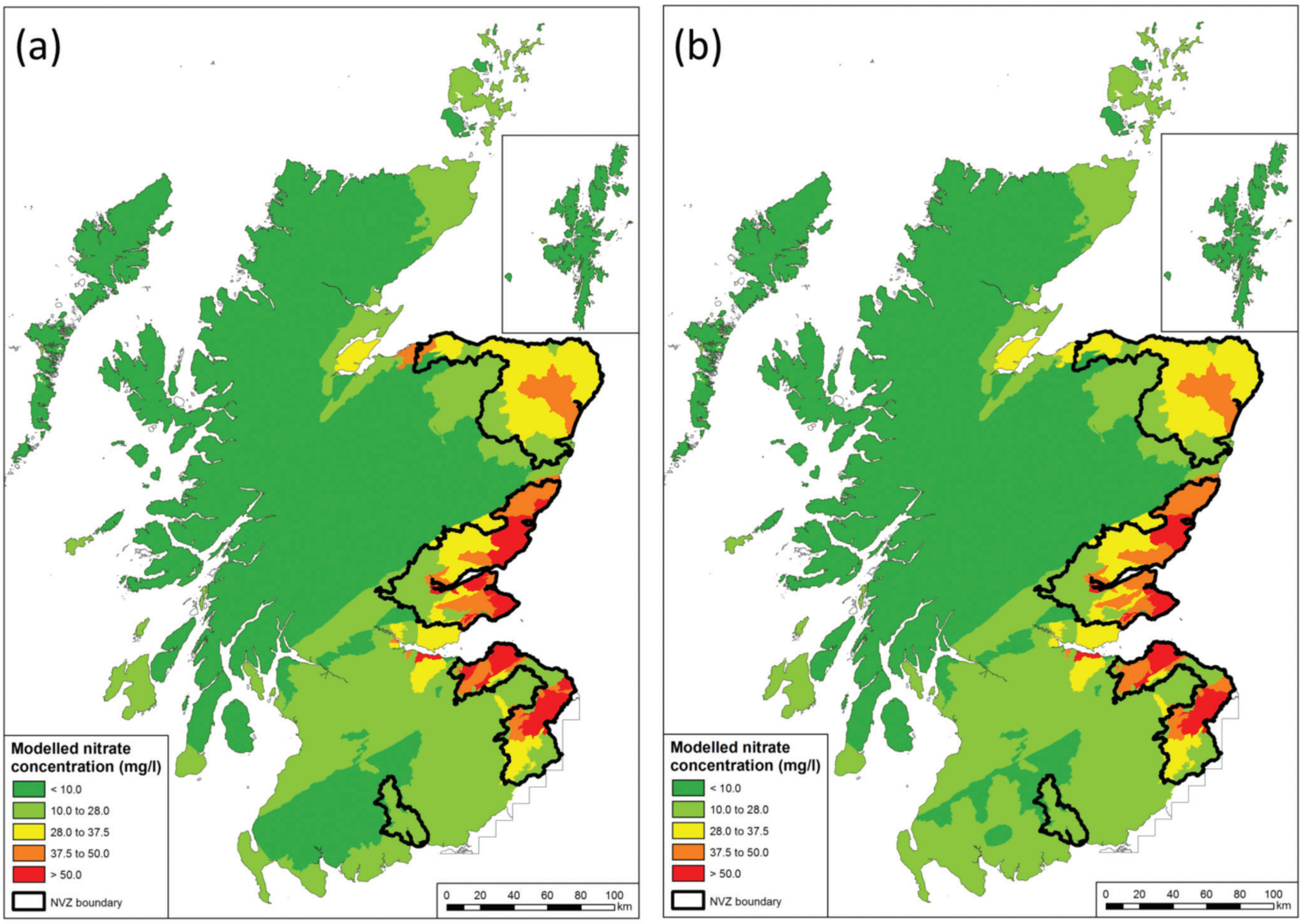

Fig. 10: Modelled nitrate concentrations for each GWB for (a) the "run 6" parameter set and (b) the "run 59" parameter set (see Table 2). Values shown are averages for the period from 2006 to 2010.

4.0 Conclusions

4.1 Objective 1

To use a physically-based, dynamic modelling approach to estimate losses of nitrate from the land to Scotland's surface and groundwaters.

- The Nitrogen Risk Assessment Model for Scotland (version 2; NIRAMS II) has been used to model nitrate concentrations at national scale for the period from 2006 to 2010.
- The model was calibrated against surface water data from the Harmonised Monitoring Scheme and then used to investigate nitrate concentrations in waters draining from the soil zone to the groundwater.

4.2 Objective 2

To demonstrate that the model is capable of adequately simulating nitrate leaching and to use it to estimate nitrate concentrations in the groundwater bodies defined under the Water Framework Directive.

- Model output has been summarised for each of the 300 groundwater bodies defined by the Water Framework Directive.
- A variety of model parameterisations provide an acceptable fit to the surface water observations. The range of output from applying these different parameter sets has been used to characterise model uncertainty.
- Although NIRAMS II does not directly simulate groundwater nitrate concentrations, in most locations there is a clear relationship between the concentrations observed in bore-holes and the modelled concentrations leaching from the soil zone.
- In most regions not associated with impermeable clays or denitrifying geology, the model's predictions are in close agreement with observed data. It is therefore reasonable to use the model to estimate nitrate losses to groundwater at ungauged locations.
- The model significantly over-predicts nitrate concentrations for six of the 42 groundwater bodies with robust monitoring data. However, these six bodies are all associated with low permeability clay layers or deep unsaturated zones, both of which inhibit the movement of pollutants from the surface to the groundwater. Some of them also have iron- and sulphur-rich bedrock geology, which leads to high rates of denitrification from within the groundwater itself. The model does not attempt to account for processes taking place below the soil zone, so there are sound physical explanations for the model's poor performance in these areas.
- Different model parameterisations produce different quantitative results, but the output is consistent when translated onto a categorical scale appropriate for the 2013 review. The results are therefore considered to be robust against uncertainties introduced by the model's parameterisation.

4.3 Objective 3

To produce maps and summaries of the model output that can be used as one strand of evidence in the 2013 Nitrates Directive review.

- Maps showing the modelled average nitrate concentration in each groundwater body have been produced for a variety of different model parameterisations. These can be used in conjunction with other lines of evidence to assess the risks to water quality from diffuse nitrate pollution.
- The model predicts high nitrate concentrations for a number of groundwater bodies located around the inner Firth of Forth that are not currently within the NVZ boundaries. However, in most of these cases the confidence in the model output is low, due to the presence of clay layers and denitrifying lithologies.
- In some areas where the model is expected to perform well, there are predictions of high nitrate concentrations in groundwater bodies that are located outside of the exiting NVZ boundaries. Conversely, some bodies within the existing boundaries are associated with low modelled concentrations. These groundwater bodies warrant more detailed consideration during the 2013 review, incorporating other strands of evidence to evaluate the overall risk to water quality.

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