Emulation of the NIRAMS model

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I. BACKGROUND

The Nitrogen Risk Assessment Model for Scotland (NIRAMS) is a nitrate leaching model. NIRAMS takes climatic inputs including rainfall and temperature, as well as chemical inputs, primarily nitrogen in various forms such as fertilizer or manure, and estimates the amount of nitrate that leaches into ground and surface waters.The NIRAMS model evaluates nitrate leaching on a grid of 485×715 one km cells that cover the whole of Scotland. Although climatic inputs are fixed to recorded values, the model includes four tunable parameters, denoted collectively by $\mathbf{x}$, that control the proportion of organic nitrogen that becomes immediately available for leaching ($\mathbf{x}_1$), the rate of mineralisation of nitrogen ($\mathbf{x}_2$), the rate of denitrification ($\mathbf{x}_3$) and the rate of nitrate leaching ($\mathbf{x}_4$) respectively. In principle these parameters can be varied independently for each one km cell and they can be tuned to match observed data, in the form of measurements of nitrate concentration in surface waters (rivers) or in ground waters (bore holes). To evaluate the NIRAMS model for the whole of Scotland, for a single set of tuning parameters and for the ten year period 2001–2010 takes approximately half an hour on a modern laptop. This high computational cost makes it difficult to repeatedly run the model for many different sets of tuning parameters in order to properly calibrate it to observed data. As input to the 2013 Nitrate Directive Review, NIRAMS was evaluated on a grid of 81 different sets of tuning parameters. The nitrate concentration in surface waters predicted by the model was compared to available observed data using a simple sum of squares difference and the set of tuning parameters that gave results closest to the observations by this measure was taken to be the representative set for further predictions.

The aim of this project was to provide more robust input to the 2017 Nitrate Directive Review by building a statistical emulator for the NIRAMS model. A statistical emulator replaces the computationally expensive simulation with a statistical model that can rapidly provide an estimate of the simulation output, with an associated uncertainty. Such an efficient emulator can then be used to properly calibrate the model, as the emulator can be quickly evaluated for many different choices of tuning parameters. In addition to providing an emulator for the first time, this work improves on previous studies by updating the climatic input to include years up to 2015 and by using ground water rather than surface water concentrations for calibration.

II. EMULATION

Given a computationally intensive process model that produces a vector of outputs, $\mathbf{y}$, given a vector of tuning parameters, $\mathbf{x}$, a statistical emulator generates an estimate of the model output, $\tilde{\mathbf{y}}_*$, at a point with arbitrary parameters, $\mathbf{x}_*$, and an estimate of the associated error in the estimate, $\delta\mathbf{y}_*$. This estimate is based on the results, $\mathbf{y}_1, \ldots \mathbf{y}_k$ of running the model at points with parameters $\mathbf{x}_1 \ldots \mathbf{x}_k$ and so it can be denoted

$$\tilde{\mathbf{y}}_* = \mathcal{E}(\mathbf{x}_*|\mathbf{x}_1 \ldots \mathbf{x}_k, \mathbf{y}_1, \ldots \mathbf{y}_k), \qquad \delta\mathbf{y}_* = \delta\mathcal{E}(\mathbf{x}_*|\mathbf{x}_1 \ldots \mathbf{x}_k, \mathbf{y}_1, \ldots \mathbf{y}_k). \tag{1}$$

Typically, evaluating the emulator will be one or more orders of magnitude cheaper than evaluating the full simulator and so the emulator can be used more readily for inference.

A. Gaussian processes

The technique we use for emulation of the NIRAMS model is Gaussian process regression. A Gaussian process is a generalisation of a Gaussian distribution to infinite numbers of dimensions. It is characterized by a mean function $m(\mathbf{x})$ and a covariance

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function $k(\mathbf{x}, \mathbf{x}')$. If $y(\mathbf{x}) \sim \mathrm{GP}(m(\mathbf{x}, k(\mathbf{x}, \mathbf{x}'))$ then at any finite set of points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ the probability distribution for the values of $y(\mathbf{x_i})$ satisfy

$$p(\mathbf{y}) \propto \exp\left[-\frac{1}{2}\sum_{ij}(x_i - m_i)K^{-1}_{ij}(x_j - m_j)\right] \tag{2}$$

where $m_i = m(\mathbf{x_i})$ and $K_{ij} = k(\mathbf{x_i}, \mathbf{x_j})$.

Gaussian processes can be used for regression if we have a training set of points at which the value of y has been measured, possible with error, i.e., we have data

$$d_i = y(\mathbf{x_i}) + \epsilon_i, \qquad \epsilon_i \sim N(0, \sigma_i^2). \tag{3}$$

The value at a new point or set of points can be found by conditioning the Gaussian process on these observed values. At a new set of points $\{\mathbf{z_i}\}$ we denote the predicted values by $y_i = y(\mathbf{z_i})$ and then

$$p(\mathbf{y}) \propto \exp\left[-\frac{1}{2}(\mathbf{y} - \mu)^T \Sigma^{-1}(\mathbf{y} - \mu)\right] \tag{4}$$

where

$$\begin{aligned}
\mu_i &= m(\mathbf{z_i}) + \sum_{jk} k(\mathbf{z_i}, \mathbf{x_j}) \left[K^{-1}\right]_{jk} (d_k - m(\mathbf{x_k})), \\
\Sigma_{ij} &= k(\mathbf{z_i}, \mathbf{z_i}) - \sum_{kl} k(\mathbf{z_i}, \mathbf{x_k}) \left[K^{-1}\right]_{kl} k(\mathbf{x_l}, \mathbf{z_j}), \\
K_{ij} &= k(\mathbf{x_i}, \mathbf{x_j}) + \sigma_i^2 \delta_{ij}.
\end{aligned} \tag{5}$$

The key thing is that the Gaussian process predicts both an expected value, $\mu(\mathbf{z_i})$, and an uncertainty, characterized by Σ, in the value of the model at a new point. This uncertainty accounts both for errors in the initial simulations (i.e., the ϵ_i's) and for uncertainty in the extrapolation from the points in parameter space where simulations have been performed, $\{\mathbf{x_i}\}$, to other points.

In any given problem, the choice of mean and covariance function for the Gaussian process are critical. It is common to use a zero mean and a squared exponential covariance function (i.e., a Gaussian). The covariance function depends on a number of free parameters which can be constrained using the set of training simulations.

Once the emulator has been constructed, if observational data, $\mathbf{d}_{\mathrm{obs}}$, is available, the emulator can be used to calibrate the model by computing the Bayesian posterior probability distribution on the tuning parameters

$$p(\mathbf{x}|\mathbf{d}_{\mathrm{obs}}) \propto p(\mathbf{d}_{\mathrm{obs}}|\mathbf{x})p(\mathbf{x}) \tag{6}$$

where $p(\mathbf{x})$ is the prior on the tuning parameters and $p(\mathbf{d}_{\mathrm{obs}}|\mathbf{x})$ is the likelihood, which is now computed using the emulator.

B. Storing the model

The output of the Gaussian process emulation needs to be stored in a convenient format to allow it to be sued for future calculations. We use HDF5 to store the results of the simulation as this is a compact binary format that allows multiple different data types to be stored and rapidly accesses. In the NIRAMS emulator files, we store various parameters describing the ground water body group for which the emulation was carried out (see below), including an identification of all one km cells within the ground waterbody group; the data used to emulate the model, the optimised parameters characterising the covariance function and the inverse of the covariance matrix $\mathbf{K}$ defined above (which allows rapid evaluation of NIRAMS output at individual new points in parameter space). When observed calibration data is available, that data is also stored in the HDF5 file, along with the posterior distribution on the tuning parameters estimated from the calibration data. The latter is stored in the form of a set of independent samples from the posterior distribution.

III. RESULTS

A. Model assumptions

For the emulation of NIRAMS, we made a number of choices. The total number of cells emulated within NIRAMS is approximately 350,000, but calibration data is only available at a small number of sites within Scotland. Some grouping of cells is therefore necessary if meaningful results are to be obtained. In the 2013 Nitrate Directive Review the grouping was whole of Scotland, i.e., a single set of tuning parameters was chosen to represent the entire country. This is clearly an oversimplification since there are a variety of different soil types, bedrock varieties and climate types within Scotland. For this work we decided to group ground water bodies into groups that had similar properties. Groupings were decided based on discussions with SEPA and we ended up with 60 ground water body groups in total. We constructed a separate emulator for each ground water body group, assuming that there was a single set of NIRAMS tuning parameters that applied to all one km cells within the ground water body group. Different ground water body groups were assumed to be independent.

NIRAMS can be used to predict daily nitrate concentrations, or the concentrations can be aggregated into monthly or annual values. Again, based on discussions with SEPA and the Scottish Government, it was decided that the relevant quantity was the six year average nitrate concentration, as this is the value used to make decisions about designation of nitrate vulnerable zones. For calibration of the model we made use of nitrate measurements in ground water from bore holes. It is known that there are significant local variations in such measurements, and so calibration data was aggregated to give an average concentration across a given ground water body group, also averaged over a 6 year period. The emulator outputs an estimated 6-year average concentration in every cell within the ground water body group, but for calibration these are averaged and compared to the observed averaged value across the ground water body group.

The emulator was constructed using a Gaussian process model as described above, with zero mean and a diagonal squared exponential covariance function. The parameters of the covariance function were chosen to maximize the evidence for the training set. While additional uncertainty comes into the model from a fixed choice of covariance function parameters, previous worked indicated there was little difference overall between using the best-fit covariance function parameters or marginalising over uncertainty in them. It was assumed that the NIRAMS output in each one km cell was an independent realisation of the same Gaussian process, but that the tuning parameters were common across all cells in the group. This is a conservative assumption.

Tuning data for the emulator was constructed by running NIRAMS on the same grid of 81 choices of tuning parameters used for the 2013 Nitrate Directive Review, but including additional data from 2010 to 2015. Climate data is fixed in this work, so predictions for the future must be based on the 6 year period between 2001 and 2015 that has the closest climate variables to what is required. Future work will explore emulation on climate variables as well.

The Gaussian process model was constructed using code written in Python and made use of the *george* Gaussian process package. Posterior distributions on tuning parameters were sampled using the *emcee* ensemble Monte Carlo sampler.

B. Emulation

An example of emulation, for the Aberdeenshire Devonian Low Load ground water body group, is shown in Figure 1. This emulator was constructed over the four tuning parameters described above and also the central year in the 6 year average. The mean value and uncertainty as estimated by the emulator are both shown in each plot. This emulator includes emulation in time, which is a proxy for the average climate input. However, the calibration data used was only for the 6 year period 2010-2015 and so only that prediction of the emulator is needed for calibration. In addition, the variation in the emulator output with year is smaller than the variation with the values of the tuning parameters and so for constraining the tuning parameters, the year variable is not needed. Therefore, for the calibration of the emulator this parameter was suppressed and emulation was only performed in the other four parameters. It is straightforward to include that parameter in the model and so emulators with year as a variable input parameter can be easily built if required. Emulators for the 2010-2015 nitrate concentration in each of the 60 ground water body groups were constructed and have been saved in the HDF5 format described above for future use. The emulator is much quicker to evaluate than the original NIRAMS model, typically taking much less than one second to provide nitrate concentrations over the whole ground water body group for any specified choice of tuning parameters.

C. Calibration

Calibration of the emulators was carried out for 48 of the 60 ground water body groups. The remaining 12 groups did not have any calibration data. An example of the calibrated emulator is shown in Figure 2. This figure shows posterior distributions in the four tuning parameters obtained using the emulator and the calibration data for the Central Fife High Load ground water body group. These results are fairly typical of the results obtained for all 48 ground water body groups. We see that the posterior distributions in the denitrification (x_3) and leaching (x_4) parameters are very flat, which indicates that these are not well constrained by the calibration data. This is consistent with the example in 1 where we see that the variation in the nitrate concentration prediction across the range of these two parameters is much smaller than the variation in the others. This suggests that these parameters are not important for obtaining reliable predictions with the NIRAMS model.

The other parameters, which determine organic nitrogen availability and the mineralisation rate, are constrained by the calibration data, as indicated by the clear peak in the posterior distribution. This is true for all ground water body groups, but the

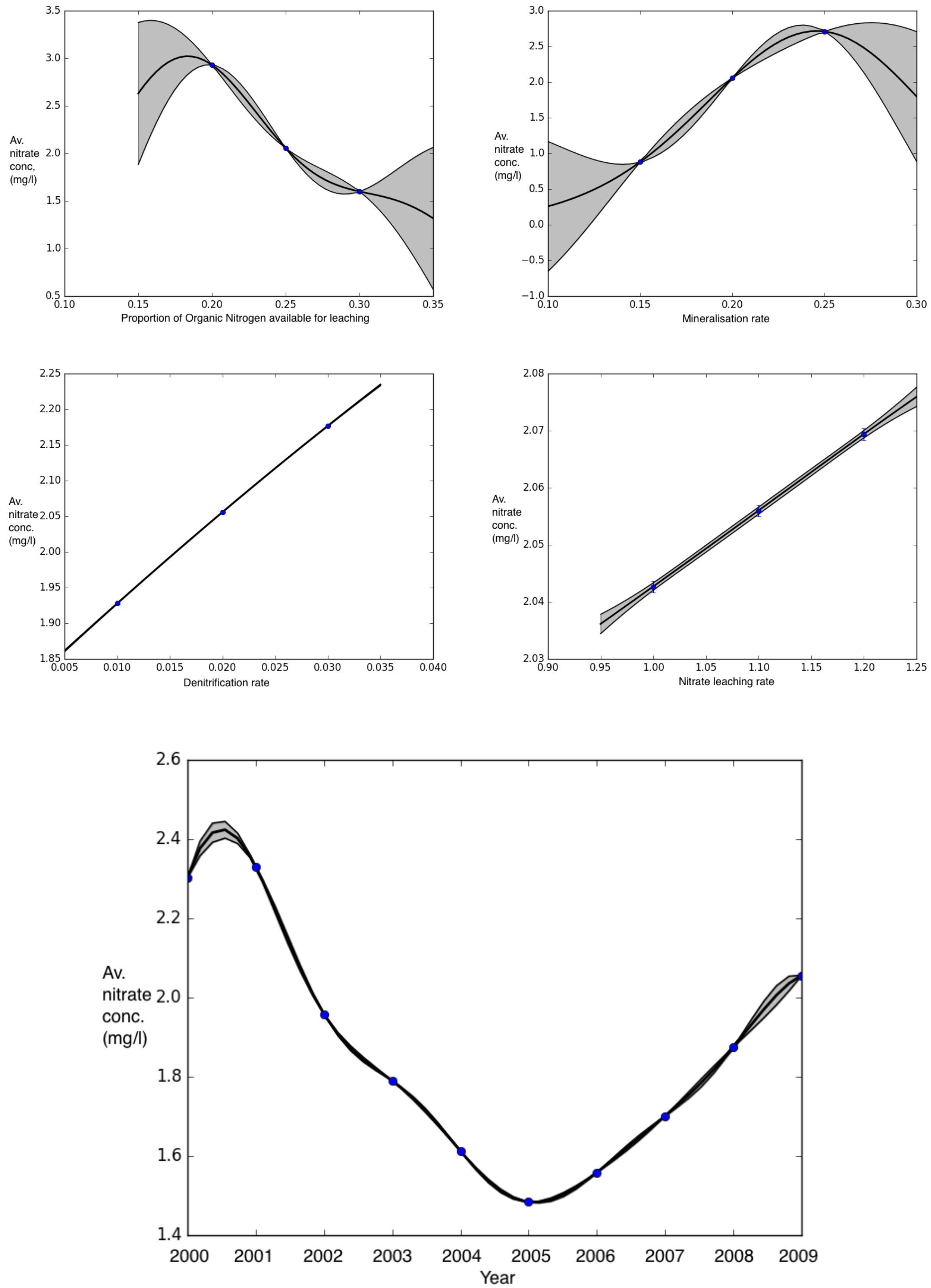

FIG. 1: Value of the 6-year average nitrate concentration, averaged over the whole of the Aberdeenshire Devonian Low Load ground water body group, as predicted by the emulator. The solid black line indicates the predicted value, and the grey shaded region is the one-sigma uncertainty region for that prediction. Blue points indicate the values computed using NIRAMS which were used for calibration of the model. Each plot shows the emulated output as a function of one of the tuning variables — x_1 (top left), x_2 (top right), x_3 (middle left), x_4 (middle right) and the central year of the 6-year average (bottom). The other parameters were fixed at the values $x_1 = 0.25$, $x_2 = 0.2$, $x_3 = 0.02$, $x_4 = 1.1$ and year = 2012 for each other figure.

location of the peaks vary from group to group, indicating that it is indeed necessary to tune these parameters separately for each ground water body group.

IV. SUMMARY AS OF DECEMBER 2017

We have generated emulators of the NIRAMS model for 60 ground water body groups in Scotland, and and calibrated the emulators using observed data for the period 2010-2015. The emulators predict the output of NIRAMS much more rapidly than running the model itself, which is what has enabled the calibration to be carried out. It would not have been possible to do the calibration of the model using NIRAMS directly. The emulators have been stored in a suitable format to be used in future work. The emulator can be used to predict the NIRAMS output for the 6 year period 2010-2015 for new choices of the tuning parameters. The calibration data can be used for future predictions - sampling from this distribution will ensure that uncertainties in the NIRAMS prediction arising from the choice of tuning parameter are properly accounted for.

One limitation in the current work is the treatment of climate variability. The climate inputs are fixed, which means that prediction under varying climate is not currently possible. Year is a proxy for those inputs, but year was ignored in the final emulator output. The code exists to generate the emulator with year as an additional variable, and this has been done for a few sample ground water body groups and could easily be extended to others. Predictions could then be based on the 6 year period within the range 2001-2015 that has the climate that most closely matches the desired climate. An alternative approach would be to include climate parameters as additional variables to be emulated. Work in this direction has begun, by introducing new parameters that scale up or down the temperature or precipitation across all the cells in a ground water body group by the same fixed amount. Construction of such an emulator requires NIRAMS to be run with modified climatic inputs to provide training data for the emulator. Such runs are being done now and then those results will be emulated to provide a tool for exploring the impact of climate change on nitrate pollution.

V. NEW RESULTS: JUNE 2018

A. Use of the emulator

The emulator provides a statistical model for the nitrate concentration in each 1km by 1km cell within each ground water body group. This takes the form of a mean concentration and an uncertainty. The mean and uncertainty are themselves dependent on the tuning parameters of the model, and calibration using observed data provides a posterior distribution on those tuning parameters. These results can be used to obtain the probability that the nitrate concentration exceeds a certain threshold. For a given choice of tuning parameters, the probability can be computed from a Gaussian distribution with the emulated mean and variance. Then these probabilities are averaged over the posterior distribution of the tuning parameters to give the final result. This can be done either for the ground water body group average nitrate concentration or for individual 1km cells within the ground water body group. In the latter case, we can combine these to compute the probability that at least one cell in the ground water body group exceeds the given threshold.

Table I summarises the results of these calculations for all ground water body groups, for the baseline scenario in which we use NIRAMS to predict the average nitrate concentration over the six year period 2010–2015. We note that for some ground water body groups no calibration data was available and so this analysis cannot be carried out. These are indicated by a line of dashes in the Table. We used thresholds of nitrate concentration of 13 mg/l, 37 mg/l and 50 mg/l based on guidance from SEPA. Figure 3 plots some of the results in this table, specifically the results in the last three columns, which are the probabilities that individual cells within the ground water body groups exceed the thresholds. Additional figures, showing the emulated mean concentration and the probabilities that the group means exceed the thresholds, are given in Appendix A.

There are a few things to note from this Table. Firstly, the probability that the group average exceeds one of these thresholds is very small in general. This is to be expected as the ground water body groups are quite spatially extensive, so the average concentration over the whole area is likely to be low. The one exception is North Fife HighLoad, for which the group average concentration has a 50% chance of exceeding the lowest threshold of 13 mg/l.

The probabilities that there are regions within the ground water body group that exceed the threshold is somewhat higher. Again this is to be expected as the 1km cells are much smaller spatially and so one might expect there to be variations on that scale within the ground water body group. For many of the ground water body groups there is still a low probability that any cell in the ground water body group would exceed the higher thresholds. However, for 31 out of the 48 groups for which calibration data is available, there is a greater than 50% chance that at least one cell in the group will exceed the low threshold of 13 mg/l. Only two ground water body groups (Easter Ross HighLoad and Moray Firth High Load) have a reasonable probability of exceeding the highest threshold of 50 mg/l somewhere in the group. Seven additional ground water body groups (Borders Sandstone Volcanics MedLoad, Central Coalfield, Central Fife HighLoad, Lothian Coalfield, Moray Firth MediumLoad, North Fife HighLoad and Strathmore Devonian HighLoad) have a greater than 1% chance of exceeding the middle threshold (37 mg/l) somewhere within the group. As we explore the impact of climate and farming practices in the following sections we will focus on these 9 ground water body groups in this report. Results are available for all groups and will be provided separately.

B. Nitrate risk under changing conditions

In this section we move away from the baseline scenario and explore the effect of varying the various inputs to the NIRAMS model. We will illustrate the various scenarios using the 9 high risk ground water body groups identified above. Figures showing the same results for all ground water body groups and comparing them between different scenarios may be found in Appendix B and Appendix C.

1. Climate variation

To explore the effect of modifications to the climate we need to move away from the fixed 2010–2015 climatic inputs used to construct the emulator for the baseline scenario. There area various ways in which this could be done. However, since the output of NIRAMS that we are emulating is an average value (the average nitrate concentration over a six year period), any spatial dependence in the climate variation that is incorporated in the model will tend to be averaged away. Therefore we adopt the simple approach of changing the temperature or precipitation by a fixed amount across all cells. To account for regional variations in rainfall, we specify a percentage modification in precipitation but an absolute modification in temperature.

For a given choice of the modified climate parameters, we can construct a new emulator for each ground water body group as described above and use this to produce the same set of summary statistics that we derived for the baseline scenario above. To calibrate the emulator we would in principle need observational data under the modified climate scenario, but that is clearly lacking. However, as the calibration data is used only to determine the appropriate values of the NIRAMS tuning parameters, it is reasonable to take the posterior distribution on those calibration parameters from the baseline scenario for any given ground water body group and use that to make predictions under the modified climate scenarios. This is the approach we take here.

We consider 8 different scenarios, which represent all combinations of a 1.5 degree temperature increase/decrease and a 50% precipitation increase/decrease. We note that this precipitation increase is very extreme, but was deliberately chosen to provide an upper bound on the level of variation. Results under each of these scenarios for the 9 high risk ground water body groups are found in Tables II–IX.

The broad conclusion from these results is that temperature changes have relatively little impact on the nitrate concentrations predicted by NIRAMS. Concentrations are slightly higher in most cases under warmer conditions and slightly lower under cooler conditions, although there are differences between different ground water body groups. Precipitation changes have a much more dramatic effect, although the 50% precipitation change represents a particularly extreme scenario. Even under this extreme scenario, the probability of exceeding 50 mg/l and 37 mg/l averaged over the ground water body group is zero for all ground water body groups. The probability of exceeding 13 mg/l would be higher compared to the other scenarios. However, under an extreme decrease in precipitation of 50%, the thresholds of both 37 mg/l and 50 mg/l are very likely to be exceeded by individual cells within the high risk ground water body groups.

2. Changing farming practices

Another impact of climate change would be to change farming practices. For example, if the weather is better farmers might leave animals on the fields for more of the year, hence increasing the deposition of manure. It is also interesting to study the impact of modifying farming practices to understand whether there are ways in which interventions could help mitigate the effects of a changing climate. In this section we demonstrate the utility of emulation for this type of work by studying the impact of modifying the organic nitrogen input to the model. This is relevant for the first example mentioned above, namely, the impact of changes to the amount of time livestock spend on the fields. As before, the approach we take to this study is to construct a separate emulator under a number of different modified organic nitrogen scenarios, and use the calibrated posterior distribution of the NIRAMS tuning parameters obtained using the baseline scenario to tune the emulator for the modified scenario.

We first consider changing the organic nitrogen input by 5%, 20% or 50%, while keeping the climate variables fixed. The results for the 9 high risk ground water body groups are summarised in Tables X–XII. Increasing the available organic nitrogen tends to increase the probability that a cell within a given ground water body group exceeds the threshold. However, this is a relatively weak effect. Even with a 50% increase in the organic nitrogen deposition the probabilities are only a few tens of percent higher.

It is also interesting to explore the combined effect of climate change and changes to organic nitrogen input. In Tables XIII–XV e show results obtained by combining a 1.5° temperature increase with each of the organic nitrogen increases. As in the

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Aberdeenshire Devonian LowLoad	—	—	—	—	—	—	—	—
Aberdeenshire Devonian MedLoad	4.380	4.265	0.0	0.0	0.0	0.2	0.0	0.0
Ayrshire Basic Rocks	—	—	—	—	—	—	—	—
Ayrshire Coalfield	—	—	—	—	—	—	—	—
Borders Carboniferous LowLoad	0.220	0.620	0.0	0.0	0.0	0.0	0.0	0.0
Borders Carboniferous MedLoad	5.670	4.923	0.0	0.0	0.0	17.2	0.0	0.0
Borders Carboniferous HighLoad	2.650	6.724	1.0	0.0	0.0	100.0	0.0	0.0
Borders LowLoad	—	—	—	—	—	—	—	—
Borders SandstoneVolcanics HighLoad	8.490	8.657	0.4	0.0	0.0	100.0	0.3	0.0
Borders SandstoneVolcanics MedLoad	3.590	4.151	0.0	0.0	0.0	100.0	6.2	0.0
Borders Sandstone MedLoad	4.310	4.680	0.0	0.0	0.0	100.0	0.0	0.0
Borders StAbbs MedLoad	6.260	6.274	0.0	0.0	0.0	100.0	0.0	0.0
Caithness Devonian	3.340	2.663	0.0	0.0	0.0	16.5	0.0	0.0
Central Coalfield	0.070	1.090	0.0	0.0	0.0	100.0	1.2	0.0
Central Fife HighLoad	5.710	6.051	0.4	0.0	0.0	100.0	5.6	0.0
Central Volcanics	1.600	1.618	0.0	0.0	0.0	94.5	0.0	0.0
Dumfries	4.960	4.691	0.0	0.0	0.0	0.3	0.0	0.0
East Lothian	3.820	6.121	0.0	0.0	0.0	100.0	0.2	0.0
Easter Ross HighLoad	3.740	3.676	0.0	0.0	0.0	100.0	39.2	11.2
Easter Ross MedLoad	3.680	3.605	0.0	0.0	0.0	97.6	0.0	0.0
Far North Devonian Sandstone	0.130	0.886	0.0	0.0	0.0	46.4	0.0	0.0
Fife Coalfield	0.110	2.180	0.0	0.0	0.0	2.3	0.0	0.0
Fife Coalfield MedLoad	0.880	2.744	0.0	0.0	0.0	99.7	0.0	0.0
Granites	—	—	—	—	—	—	—	—
Highland Tertiary volcanics	0.230	0.498	0.0	0.0	0.0	0.0	0.0	0.0
Highlands and Islands	1.290	1.334	0.0	0.0	0.0	100.0	0.2	0.0
Karst limestone	—	—	—	—	—	—	—	—
Lewis Permian	—	—	—	—	—	—	—	—
Lochar Moss	4.780	4.042	0.0	0.0	0.0	0.5	0.0	0.0
Lothian Coalfield	0.070	5.399	0.0	0.0	0.0	100.0	1.1	0.0
Mined Carboniferous	—	—	—	—	—	—	—	—
Moray Firth MediumLoad	1.000	4.864	2.0	0.0	0.0	100.0	48.5	0.6
Moray Firth HighLoad	9.600	9.372	0.5	0.0	0.0	100.0	49.9	9.9
Nithsdale LowLoad	—	—	—	—	—	—	—	—
Nithsdale MedLoad	2.410	2.491	0.0	0.0	0.0	0.0	0.0	0.0
Non Coal Carboniferous	1.830	1.885	0.0	0.0	0.0	69.2	0.0	0.0
North Fife HighLoad	13.260	12.838	52.7	0.0	0.0	100.0	20.3	0.0
North Fife MedLoad	—	—	—	—	—	—	—	—
Passage Formation	0.070	1.499	0.0	0.0	0.0	3.7	0.0	0.0
Passage Formation MedLoad	0.070	4.683	0.0	0.0	0.0	82.5	0.0	0.0
Permian Basin	0.710	1.198	0.0	0.0	0.0	0.0	0.0	0.0
Sanquhar Coalfield	—	—	—	—	—	—	—	—
Shetland Low Permeability	0.450	0.675	0.0	0.0	0.0	2.5	0.0	0.0
Silurian Ordovician	2.640	2.488	0.0	0.0	0.0	100.0	0.0	0.0
Solway MedLoad	3.010	3.094	0.0	0.0	0.0	1.6	0.0	0.0
South Fife LowKsuperficial HighLoad	1.340	5.762	0.1	0.0	0.0	100.0	0.0	0.0
South Fife LowKsuperficial MedLoad	1.890	2.732	0.0	0.0	0.0	25.4	0.0	0.0
Southern Devonian	6.240	5.365	0.0	0.0	0.0	100.0	0.0	0.0
Southern Highlands	1.210	1.141	0.0	0.0	0.0	94.0	0.0	0.0
Southern Highlands MediumLoad	3.850	4.053	0.0	0.0	0.0	100.0	0.0	0.0
Southern Highlands HighLoad	7.160	7.206	0.9	0.0	0.0	100.0	0.7	0.0
Stewartry Coastal	12.750	7.886	0.0	0.0	0.0	100.0	0.0	0.0
Stranraer	6.860	6.216	0.0	0.0	0.0	100.0	0.0	0.0
Strathmore Devonian HighLoad	8.690	8.387	0.2	0.0	0.0	100.0	27.7	0.0
Strathmore Devonian LowKsuperficial	5.880	6.030	0.0	0.0	0.0	100.0	0.0	0.0
Strathmore Devonian LowLoad	1.710	1.685	0.0	0.0	0.0	7.3	0.0	0.0
Strathmore Devonian MedLoad	1.300	3.074	0.0	0.0	0.0	98.2	0.0	0.0
Thornhill	6.480	3.434	0.0	0.0	0.0	0.0	0.0	0.0
Turriff	7.990	7.814	0.0	0.0	0.0	100.0	0.0	0.0
West Lothian Carboniferous MedLoad	—	—	—	—	—	—	—	—

TABLE I: Emulator results for each ground water body group. The columns give the ground water body group name, the measured averaged concentration in the period 2010–2015 used to calibrate the model, the emulated average concentration (computed by averaging over the posterior on the tuning parameters) and the probabilities that the average concentration in the ground water body group exceeds various thresholds (columns 4–6) or the concentration in at least one 1km cell in the ground water body group exceeds the same thresholds (columns 7–9). Thresholds of 13, 37 and 50 mg/l were used. Probabilities are expressed as percentages. Rows of the table that are all dashes indicate the 12 groups for which no calibration data was available.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	4.497	0.0	0.0	0.0	100.0	4.4	0.0
Central Coalfield	0.070	1.308	0.0	0.0	0.0	100.0	2.5	0.0
Central Fife HighLoad	5.710	6.507	0.8	0.0	0.0	100.0	5.3	0.0
Easter Ross HighLoad	3.740	3.924	0.0	0.0	0.0	100.0	35.9	7.4
Lothian Coalfield	0.070	5.607	0.0	0.0	0.0	100.0	0.3	0.0
Moray Firth MediumLoad	1.000	5.788	8.0	0.0	0.0	100.0	96.5	13.8
MorayFirth HighLoad	9.600	9.364	0.3	0.0	0.0	100.0	48.4	5.9
North Fife HighLoad	13.260	12.808	50.2	0.0	0.0	100.0	10.0	0.0
Strathmore Devonian HighLoad	8.690	8.784	0.3	0.0	0.0	100.0	12.2	0.0

TABLE II: Group average concentrations and probabilities that the group average or at least one individual cell exceeds the various nitrate thresholds, under a scneario in which the temperature is increased by 1.5° while precipitation is left unchanged. The meaning of each column is as for Table I.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	4.406	0.0	0.0	0.0	100.0	3.9	0.0
Central Coalfield	0.070	1.306	0.0	0.0	0.0	100.0	4.0	0.0
Central Fife HighLoad	5.710	6.510	0.9	0.0	0.0	100.0	5.3	0.0
Easter Ross HighLoad	3.740	3.746	0.0	0.0	0.0	100.0	33.5	6.4
Lothian Coalfield	0.070	5.620	0.0	0.0	0.0	100.0	0.1	0.0
Moray Firth MediumLoad	1.000	5.481	3.7	0.0	0.0	100.0	82.0	2.8
Moray Firth HighLoad	9.600	9.002	0.2	0.0	0.0	100.0	42.5	4.4
North Fife HighLoad	13.260	12.218	27.0	0.0	0.0	100.0	4.8	0.0
Strathmore Devonian HighLoad	8.690	8.354	0.0	0.0	0.0	100.0	6.3	0.0

TABLE III: As Table II, but now for a scenario in which temperature decreases by 1.5°.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	2.395	0.0	0.0	0.0	47.3	0.0	0.0
Central Coalfield	0.070	0.638	0.0	0.0	0.0	18.9	0.0	0.0
Central Fife HighLoad	5.710	2.951	0.0	0.0	0.0	11.4	0.0	0.0
Easter Ross HighLoad	3.740	1.740	0.0	0.0	0.0	35.5	0.0	0.0
Lothian Coalfield	0.070	1.887	0.0	0.0	0.0	0.1	0.0	0.0
Moray Firth MediumLoad	1.000	2.642	0.0	0.0	0.0	100.0	0.0	0.0
Moray Firth HighLoad	9.600	4.915	0.0	0.0	0.0	92.4	0.0	0.0
North Fife HighLoad	13.260	4.679	0.0	0.0	0.0	5.5	0.0	0.0
Strathmore Devonian HighLoad	8.690	3.979	0.0	0.0	0.0	30.1	0.0	0.0

TABLE IV: As Table II, but now for a scenario in which the temperature is unchanged, but precipitation increases by 50%.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	10.239	11.7	0.0	0.0	100.0	99.7	83.7
Central Coalfield	0.070	3.664	0.0	0.0	0.0	100.0	100.0	51.7
Central Fife HighLoad	5.710	13.246	32.1	0.0	0.0	100.0	99.9	91.5
Easter Ross HighLoad	3.740	5.060	0.0	0.0	0.0	100.0	79.6	37.3
Lothian Coalfield	0.070	11.167	7.3	0.0	0.0	100.0	77.0	1.0
Moray Firth MediumLoad	1.000	5.723	0.1	0.0	0.0	100.0	53.1	8.9
Moray Firth HighLoad	9.600	7.354	0.0	0.0	0.0	100.0	0.0	0.0
North Fife HighLoad	13.260	13.707	71.8	0.0	0.0	100.0	83.4	7.5
Strathmore Devonian HighLoad	8.690	16.641	97.9	0.0	0.0	100.0	100.0	100.0

TABLE V: As Table II, but now for a scenario in which the temperature is unchanged but precipitation decreases by 50%.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	2.352	0.0	0.0	0.0	43.7	0.0	0.0
Central Coalfield	0.070	0.640	0.0	0.0	0.0	20.1	0.0	0.0
Central Fife HighLoad	5.710	3.012	0.0	0.0	0.0	16.2	0.0	0.0
Easter Ross HighLoad	3.740	1.787	0.0	0.0	0.0	42.3	0.0	0.0
Lothian Coalfield	0.070	1.876	0.0	0.0	0.0	0.1	0.0	0.0
Moray Firth MediumLoad	1.000	2.628	0.0	0.0	0.0	100.0	0.0	0.0
Moray Firth HighLoad	9.600	5.075	0.0	0.0	0.0	95.4	0.0	0.0
North Fife HighLoad	13.260	4.779	0.0	0.0	0.0	8.5	0.0	0.0
Strathmore Devonian HighLoad	8.690	4.066	0.0	0.0	0.0	36.1	0.0	0.0

TABLE VI: As Table II, but now for a scenario in which temperature increases by 1.5° and precipitation increases by 50%.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	2.382	0.0	0.0	0.0	48.2	0.0	0.0
Central Coalfield	0.070	0.645	0.0	0.0	0.0	14.4	0.0	0.0
Central Fife HighLoad	5.710	2.902	0.0	0.0	0.0	6.5	0.0	0.0
Easter Ross HighLoad	3.740	1.693	0.0	0.0	0.0	27.3	0.0	0.0
Lothian Coalfield	0.070	1.877	0.0	0.0	0.0	0.0	0.0	0.0
Moray Firth MediumLoad	1.000	2.562	0.0	0.0	0.0	100.0	0.0	0.0
Moray Firth HighLoad	9.600	4.687	0.0	0.0	0.0	83.5	0.0	0.0
North Fife HighLoad	13.260	4.517	0.0	0.0	0.0	2.1	0.0	0.0
Strathmore Devonian HighLoad	8.690	3.897	0.0	0.0	0.0	25.2	0.0	0.0

TABLE VII: As Table II, but now for a scenario in which temperature decreases by 1.5° and precipitation increases by 50%.

previous section, we find that the temperature increase has a weak effect, which depends on the ground water body group, although the tendency is to slightly increase the probability of thresholds being exceeded.

VI. SUMMARY AND FUTURE PLANS

We have used the emulator to explore in detail a range of different scenarios for climate and farming practices. There are a few avenues for further investigation that could be explored in the future. Firstly, we have considered only modifications to the organic nitrogen input, but NIRAMS also specifies other sources of nitrogen input and so it might be interesting to explore the impact of those on the results. These inputs are related to farming practices, so exploring what happens as these other inputs are varied could help us understand how regulation might mitigate some of the impacts of climate change. Secondly, we have only considered a few discrete climate change scenarios and it would be informative to consider a wider range of choices for temperature and precipitation changes. Finally, the way in which the climate change modifications were imposed was simplistic — a fixed absolute temperature change and a fixed fractional precipitation change. It might be interesting to explore if including changes in climate seasonality (e.g., wetter winters and drier summers) has any impact on the results.

The exploration of a wide range of climate scenarios will be facilitated by the development of an emulator that takes as input parameters not only the NIRAMS tuning parameters but also parameters that characterise the climate and farming practices.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	10.504	11.9	0.0	0.0	100.0	99.8	88.3
Central Coalfield	0.070	3.773	0.0	0.0	0.0	100.0	100.0	69.6
Central Fife HighLoad	5.710	13.221	29.0	0.1	0.0	100.0	99.9	94.9
Easter Ross HighLoad	3.740	4.926	0.0	0.0	0.0	100.0	71.8	30.2
Lothian Coalfield	0.070	11.193	7.9	0.0	0.0	100.0	75.8	0.5
Moray Firth MediumLoad	1.000	5.663	0.1	0.0	0.0	100.0	48.0	7.8
Moray Firth HighLoad	9.600	7.376	0.0	0.0	0.0	100.0	0.1	0.0
North Fife HighLoad	13.260	13.595	68.8	0.0	0.0	100.0	78.8	6.6
Strathmore Devonian HighLoad	8.690	16.113	96.7	0.0	0.0	100.0	100.0	99.9

TABLE VIII: As Table II, but now for a scenario in which temperature increases by 1.5° and precipitation decreases by 50%.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	10.046	10.7	0.0	0.0	100.0	99.4	76.9
Central Coalfield	0.070	3.570	0.0	0.0	0.0	100.0	100.0	87.7
Central Fife HighLoad	5.710	13.466	35.8	0.0	0.0	100.0	99.9	88.4
Easter Ross HighLoad	3.740	5.448	0.0	0.0	0.0	100.0	82.7	43.0
Lothian Coalfield	0.070	11.313	9.2	0.0	0.0	100.0	93.9	8.5
Moray Firth MediumLoad	1.000	5.867	0.1	0.0	0.0	100.0	62.1	10.5
Moray Firth HighLoad	9.600	7.468	0.0	0.0	0.0	100.0	0.1	0.0
North Fife HighLoad	13.260	14.470	87.2	0.0	0.0	100.0	95.7	13.6
Strathmore Devonian HighLoad	8.690	17.566	99.0	0.0	0.0	100.0	100.0	100.0

TABLE IX: As Table II, but now for a scenario in which temperature decreases by 1.5° and precipitation decreases by 50%.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	4.953	0.0	0.0	0.0	100.0	0.0	0.0
Central Coalfield	0.070	1.508	0.0	0.0	0.0	100.0	0.0	0.0
Central Fife HighLoad	5.710	7.588	1.8	0.0	0.0	100.0	8.2	0.0
Easter Ross HighLoad	3.740	4.509	0.0	0.0	0.0	100.0	44.5	2.5
Lothian Coalfield	0.070	8.138	10.3	0.0	0.0	100.0	32.6	0.0
Moray Firth MediumLoad	1.000	6.163	1.0	0.0	0.0	100.0	54.6	0.9
Moray Firth HighLoad	9.600	8.018	8.2	0.0	0.0	100.0	26.8	0.1
North Fife HighLoad	13.260	9.398	10.9	0.0	0.0	100.0	0.3	0.0
Strathmore Devonian HighLoad	8.690	7.729	2.4	0.0	0.0	100.0	16.1	0.0

TABLE X: Group average concentrations and probabilities that the group average or at least one individual cell exceeds the various nitrate thresholds, under a scenario in which the climate is unchanged, but the amount of organic nitrogen input is increased by 5%. The meaning of each column is as for Table I.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	4.996	0.0	0.0	0.0	100.0	0.0	0.0
Central Coalfield	0.070	1.528	0.0	0.0	0.0	100.0	0.0	0.0
Central Fife HighLoad	5.710	7.643	2.2	0.0	0.0	100.0	9.4	0.0
Easter Ross HighLoad	3.740	4.492	0.0	0.0	0.0	100.0	45.1	2.5
Lothian Coalfield	0.070	8.262	11.4	0.0	0.0	100.0	37.4	0.0
Moray Firth MediumLoad	1.000	6.280	1.8	0.0	0.0	100.0	66.8	1.7
Moray Firth HighLoad	9.600	8.071	9.5	0.0	0.0	100.0	31.0	0.1
North Fife HighLoad	13.260	9.404	11.6	0.0	0.0	100.0	0.5	0.0
Strathmore Devonian HighLoad	8.690	7.844	2.3	0.0	0.0	100.0	15.4	0.0

TABLE XI: As Table X, but now for a scenario in which the amount of organic nitrogen input is increased by 20%.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	5.221	0.0	0.0	0.0	100.0	0.0	0.0
Central Coalfield	0.070	1.578	0.0	0.0	0.0	100.0	0.2	0.0
Central Fife HighLoad	5.710	7.720	1.8	0.0	0.0	100.0	9.3	0.0
Easter Ross HighLoad	3.740	4.609	0.0	0.0	0.0	100.0	53.8	3.3
Lothian Coalfield	0.070	8.574	12.7	0.0	0.0	100.0	43.1	0.0
Moray Firth MediumLoad	1.000	6.517	2.1	0.0	0.0	100.0	80.8	3.4
Moray Firth HighLoad	9.600	8.342	9.4	0.0	0.0	100.0	40.7	0.4
North Fife HighLoad	13.260	9.484	11.9	0.0	0.0	100.0	1.3	0.0
Strathmore Devonian HighLoad	8.690	8.048	3.3	0.0	0.0	100.0	20.3	0.0

TABLE XII: As Table X, but now for a scenario in which the amount of organic nitrogen input is increased by 50%.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	4.959	0.0	0.0	0.0	100.0	0.0	0.0
Central Coalfield	0.070	1.506	0.0	0.0	0.0	100.0	0.0	0.0
Central Fife HighLoad	5.710	7.573	2.4	0.0	0.0	100.0	12.3	0.0
Easter Ross HighLoad	3.740	4.564	0.0	0.0	0.0	100.0	40.5	1.8
Lothian Coalfield	0.070	8.237	10.9	0.0	0.0	100.0	36.2	0.0
Moray Firth MediumLoad	1.000	6.154	1.1	0.0	0.0	100.0	54.8	0.8
Moray Firth HighLoad	9.600	8.063	8.3	0.0	0.0	100.0	25.9	0.2
North Fife HighLoad	13.260	9.384	12.1	0.0	0.0	100.0	0.1	0.0
Strathmore Devonian HighLoad	8.690	7.807	2.5	0.0	0.0	100.0	15.7	0.0

TABLE XIII: As Table X, but now for a scenario in which the temperature is increased by 1.5°, and the amount of organic nitrogen input is increased by 5%.

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	5.055	0.0	0.0	0.0	100.0	0.0	0.0
Central Coalfield	0.070	1.548	0.0	0.0	0.0	100.0	0.0	0.0
Central Fife HighLoad	5.710	7.660	2.2	0.0	0.0	100.0	10.3	0.0
Easter Ross HighLoad	3.740	4.575	0.0	0.0	0.0	100.0	44.5	2.4
Lothian Coalfield	0.070	8.303	11.6	0.0	0.0	100.0	40.1	0.0
Moray Firth MediumLoad	1.000	6.273	1.3	0.0	0.0	100.0	59.6	0.9
Moray Firth HighLoad	9.600	7.985	7.6	0.0	0.0	100.0	24.1	0.3
North Fife HighLoad	13.260	9.494	12.3	0.0	0.0	100.0	0.5	0.0
Strathmore Devonian HighLoad	8.690	7.920	2.7	0.0	0.0	100.0	15.5	0.0

TABLE XIV: As Table X, but now for a scenario in which the temperature is increased by 1.5°, and the amount of organic nitrogen input is increased by 20%.

Some initial work has started in this direction. An initial emulator has been produced and works, but it is not as precise as it could be. The emulator used a fixed covariance structure to characterise the dependence on the tuning parameters across all climates and that appears to be a poor model - adding the climate variables thus inflates the uncertainty for the baseline scenario. This problem should be mitigated by using a more complex structure for the Gaussian process model that adapts the covariance structure as a function of the climate variables. An exploration of this is currently underway and we hope to have a generic emulator available in the near future.

Appendix A: Additional figures: baseline

In this appendix we provide some additional figures for the baseline scenario, i.e., the NIRAMS prediction for the average nitrate concentration over the 6 year period 2010–2015. In Figure 4 we

Ground water body group	Measured Conc.	Emulated Conc.	Prob. group av. conc. exceeds			Prob. conc. in cell exceeds		
			13 mg/l	37 mg/l	50 mg/l	13 mg/l	37 mg/l	50 mg/l
Borders SandstoneVolcanics MedLoad	3.590	5.233	0.0	0.0	0.0	100.0	0.1	0.0
Central Coalfield	0.070	1.599	0.0	0.0	0.0	100.0	0.1	0.0
Central Fife HighLoad	5.710	7.736	2.6	0.0	0.0	100.0	13.4	0.0
Easter Ross HighLoad	3.740	4.679	0.0	0.0	0.0	100.0	52.7	4.0
Lothian Coalfield	0.070	8.652	12.5	0.0	0.0	100.0	45.9	0.1
Moray Firth MediumLoad	1.000	6.622	2.1	0.0	0.0	100.0	77.1	2.3
Moray Firth HighLoad	9.600	8.573	10.7	0.0	0.0	100.0	38.3	0.6
North Fife HighLoad	13.260	9.623	13.7	0.0	0.0	100.0	2.9	0.0
Strathmore Devonian HighLoad	8.690	8.162	4.0	0.0	0.0	100.0	20.5	0.0

TABLE XV: As Table X, but now for a scenario in which the temperature is increased by 1.5°, and the amount of organic nitrogen input is increased by 50%.

Appendix B: Additional figures: nitrate risk under climate variation

In this appendix we provide figures summarising the results of the various modified climate scenarios presented in section V B 1. Each Figure has multiple panels, which represent different modifications to the conditions. The labelling of the scenarios is as follows

(a) Temperature increase by $1.5°$;

(b) Temperature decrease by $1.5°$;

(c) Precipitation increase by 50%;

(d) Precipitation decrease by 50%;

(e) Temperature increase by $1.5°$ and precipitation increase by 50%;

(f) Temperature decrease by $1.5°$ and precipitation increase by 50%;

(g) Temperature increase by $1.5°$ and precipitation decrease by 50%;

(h) Temperature decrease by $1.5°$ and precipitation decrease by 50%;

1. Mean concentrations

In Figure 6 we show the mean nitrate concentration for each ground water body group, under each of the modified climate scenarios listed above.

2. Probability that group average exceeds threshold

In Figures 7–9 we show the probability that the average concentration in a given ground water body group exceeds the specified nitrate threshold. Results are shown for each of the climate change scenarios listed previously. Figure 7 shows results for a threshold of 13 mg/l, Figures 8 for a threshold of 37 mg/l and Figures 9 for a threshold of 50 mg/l.

3. Probability that cells within group exceed threshold

In Figures 10–12 we show the probability that the concentration in at least one cell within any given ground water body group exceeds the specified nitrate threshold. Results are shown for each of the climate change scenarios listed previously. Figure 10 shows results for a threshold of 13 mg/l, Figures 11 for a threshold of 37 mg/l and Figures 12 for a threshold of 50 mg/l.

Appendix C: Additional figures: nitrate risk under changing farming practices

n this appendix we provide figures summarising the results of the various modified nitrogen input scenarios presented in section V B 2. Each Figure has multiple panels, which represent different modifications to the conditions. The labelling of the scenarios is as follows

(a) Increase in organic nitrogen inputs by 5%;

(b) Increase in organic nitrogen inputs by 20%;

(c) Increase in organic nitrogen inputs by 50%;

(d) Temperature increase by $1.5°$ and increase in organic nitrogen inputs by 5%;

(e) Temperature increase by $1.5°$ and increase in organic nitrogen inputs by 20%;

(f) Temperature increase by $1.5°$ and increase in organic nitrogen inputs by 50%.

1. Mean concentrations

In Figure 13 we show the mean nitrate concentration for each ground water body group, under each of the modified organic nitrogen scenarios listed above.

2. Probability that group average exceeds threshold

In Figures 14–16 we show the probability that the average concentration in a given ground water body group exceeds the specified nitrate threshold. Results are shown for each of the organic nitrogen scenarios listed previously. Figure 14 shows results for a threshold of 13 mg/l, Figures 15 for a threshold of 37 mg/l and Figures 16 for a threshold of 50 mg/l.

3. Probability that cells within group exceed threshold

In Figures 17–19 we show the probability that the concentration in at least one cell within any given ground water body group exceeds the specified nitrate threshold. Results are shown for each of the organic nitrogen scenarios listed previously. Figure 17 shows results for a threshold of 13 mg/l, Figures 18 for a threshold of 37 mg/l and Figures 19 for a threshold of 50 mg/l.

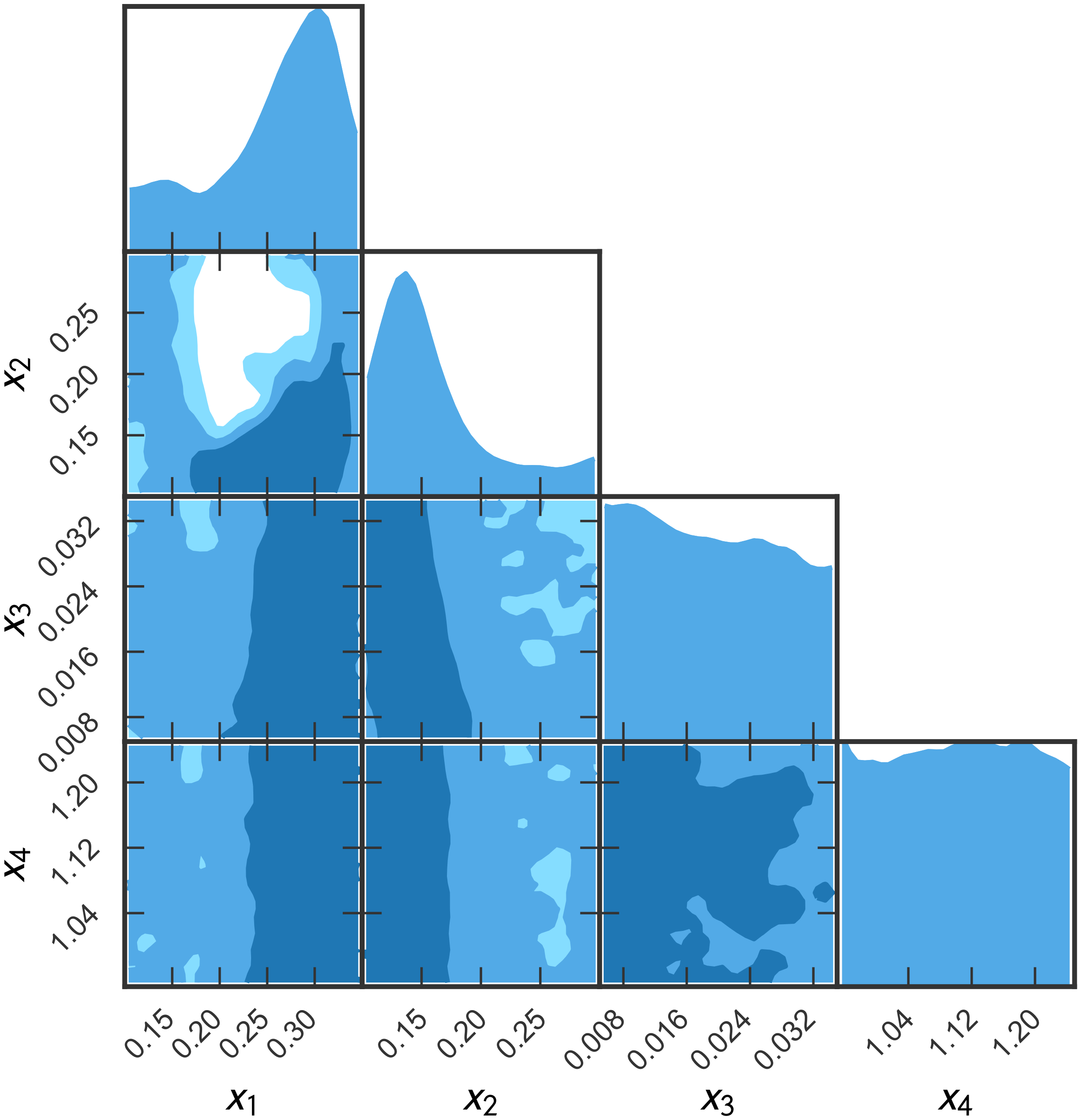

FIG. 2: Posterior distributions on the four NIRAMS tuning parameters for the Central Fife High Load ground water body group. We show two-dimensional marginalised posterior distributions for each pair of tuning parameters and, at the top of each column, the 1D marginalised posterior distribution for the column parameter. The four parameters characterise the proportion of organic nitrogen that becomes immediately available for leaching ($\mathbf{x}_1$), the rate of mineralisation of nitrogen ($\mathbf{x}_2$), the rate of denitrification ($\mathbf{x}_3$) and the rate of nitrate leaching ($\mathbf{x}_4$) respectively. In the 2D plots, the dark, medium and light blue regions denote 68%, 95% and 99% confidence regions respectively. White regions lis outside the 99% contour..

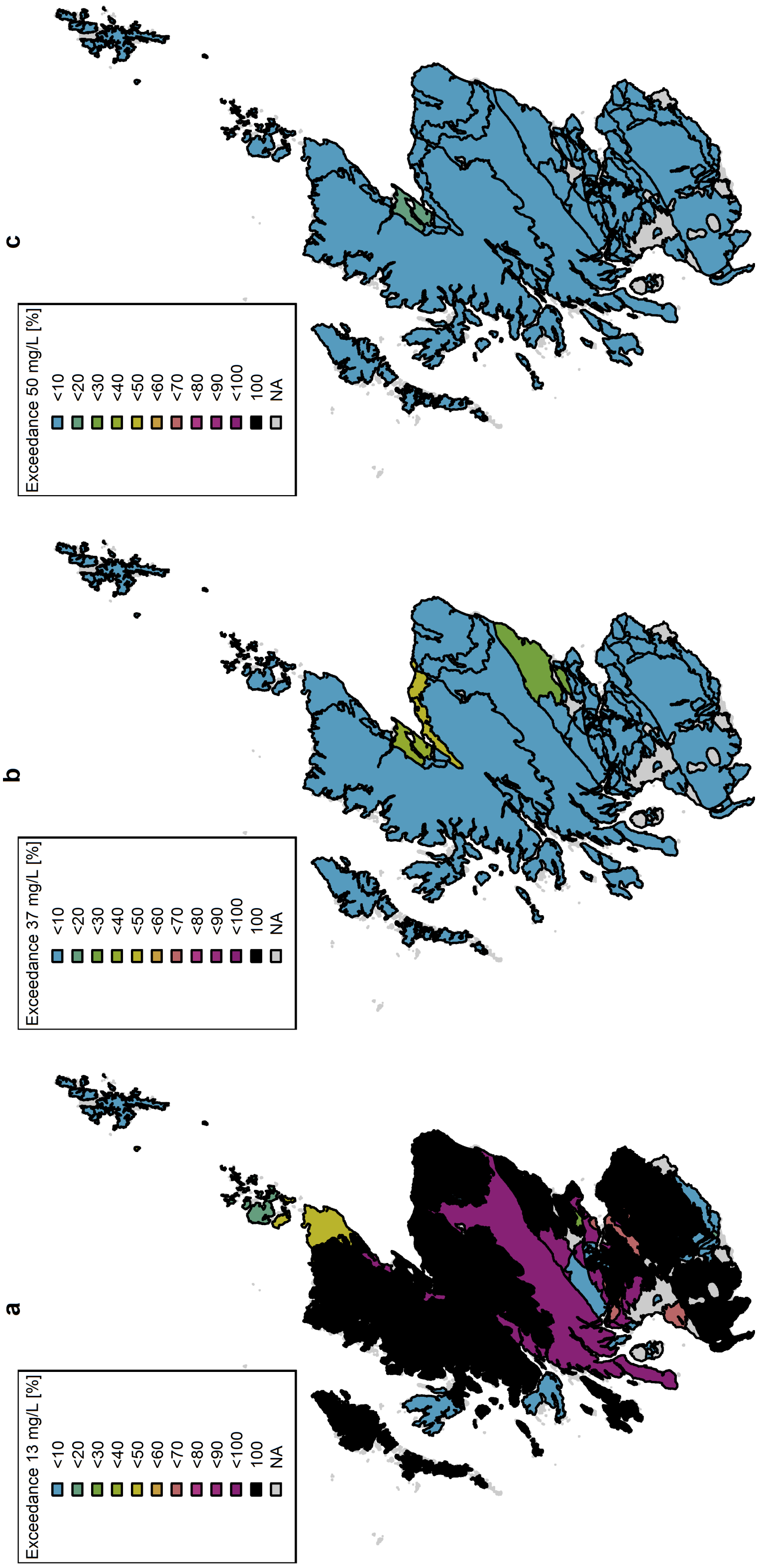

FIG. 3: Probability that the average nitrate concentration in each ground water body group exceeds the three nitrate thresholds — 13 mg/l (panel a), 37 mg/l (panel b) or 50 mg/l (panel c). This is for the baseline scenario predicting the 6 year average concentration over 2010–2015 using fixed climatic inputs.

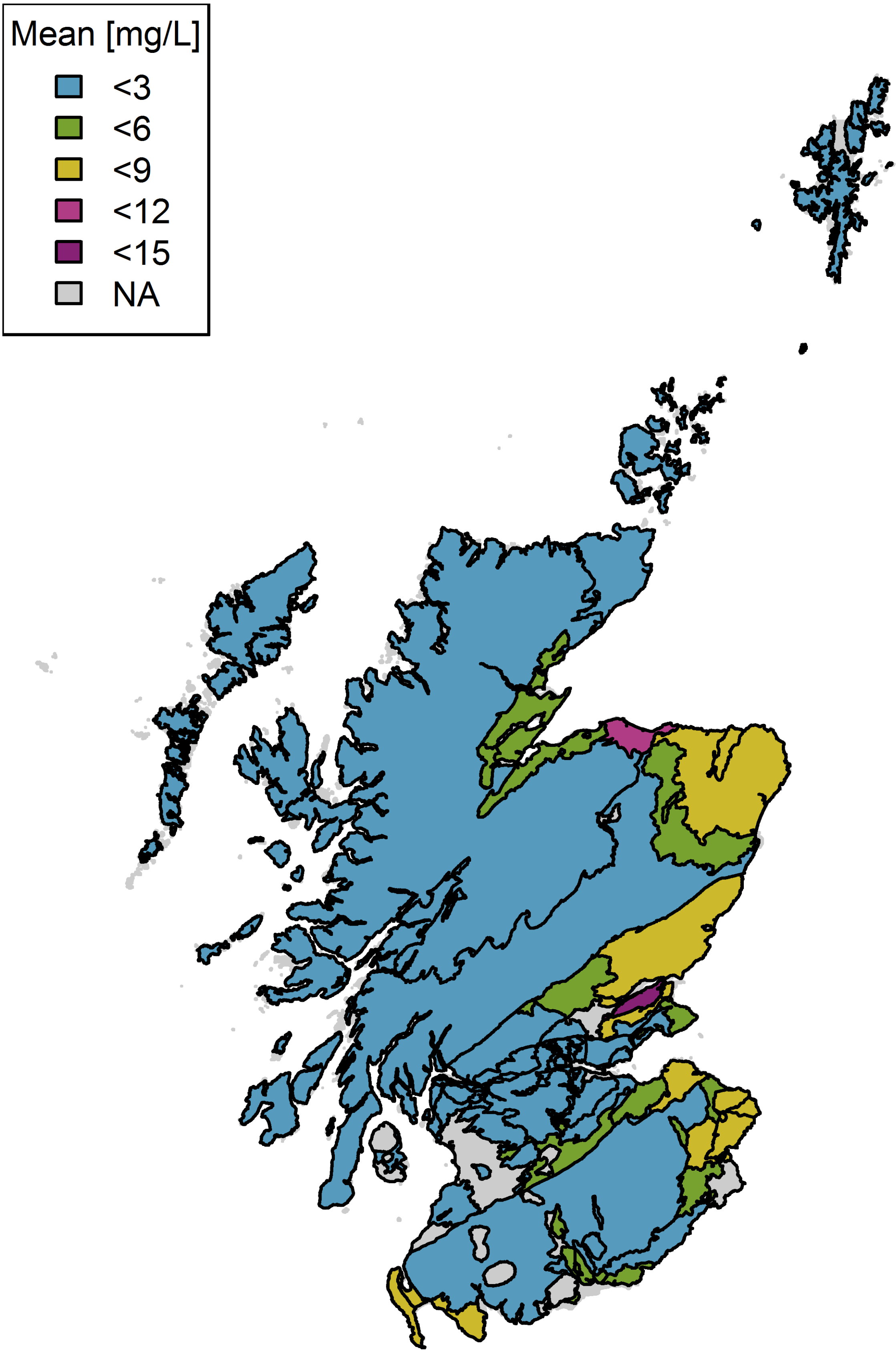

FIG. 4: Mean nitrate concentration in each ground water body group, as predicted by the emulator. This is for the baseline scenario predicting the 6 year average concentration over 2010–2015 using fixed climatic inputs.

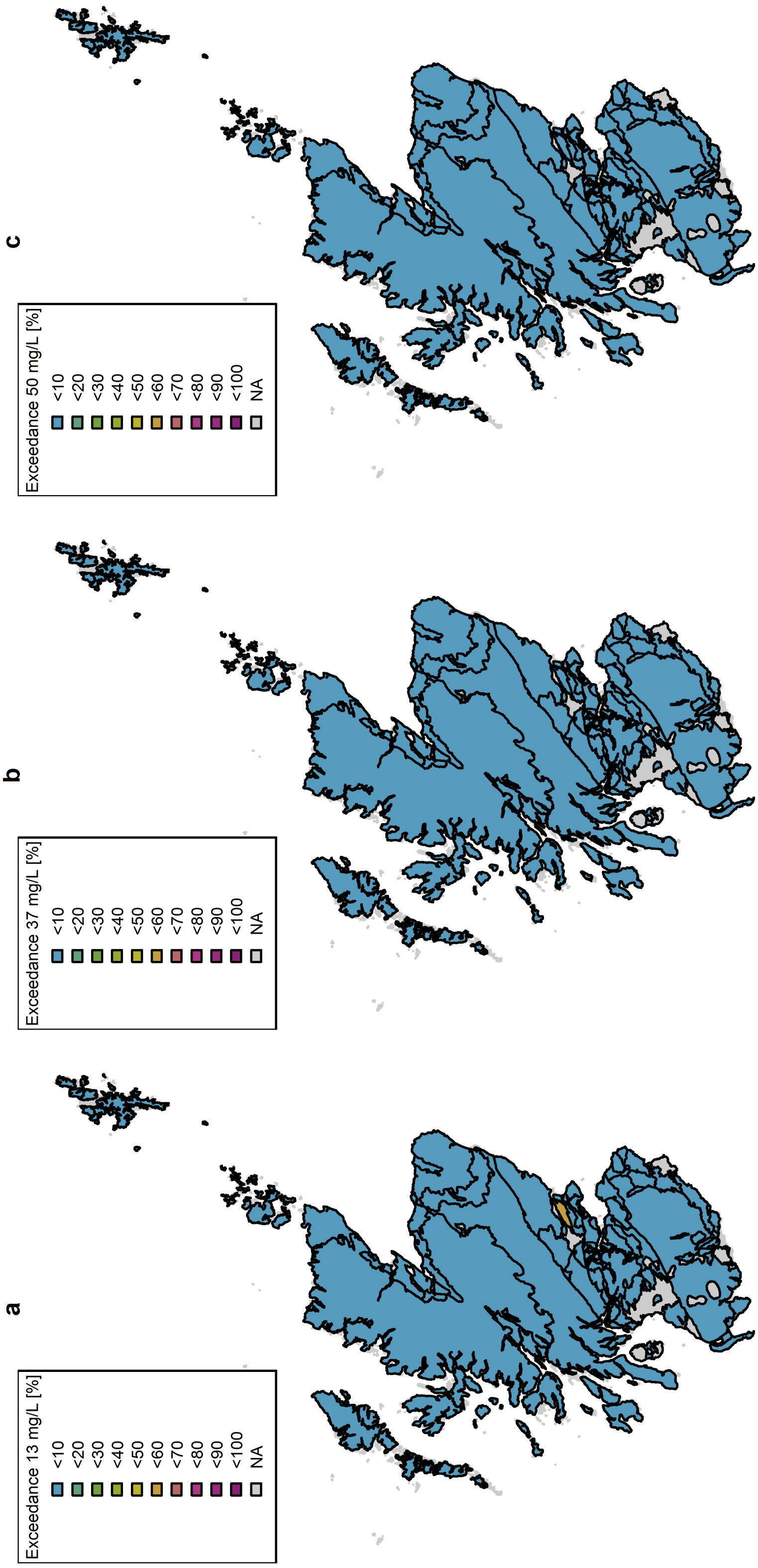

FIG. 5: Probability that the average nitrate concentration in each ground water body group exceeds the three nitrate thresholds — 13 mg/l (panel a), 37 mg/l (panel b) or 50 mg/l (panel c). This is for the baseline scenario predicting the 6 year average concentration over 2010–2015 using fixed climatic inputs.

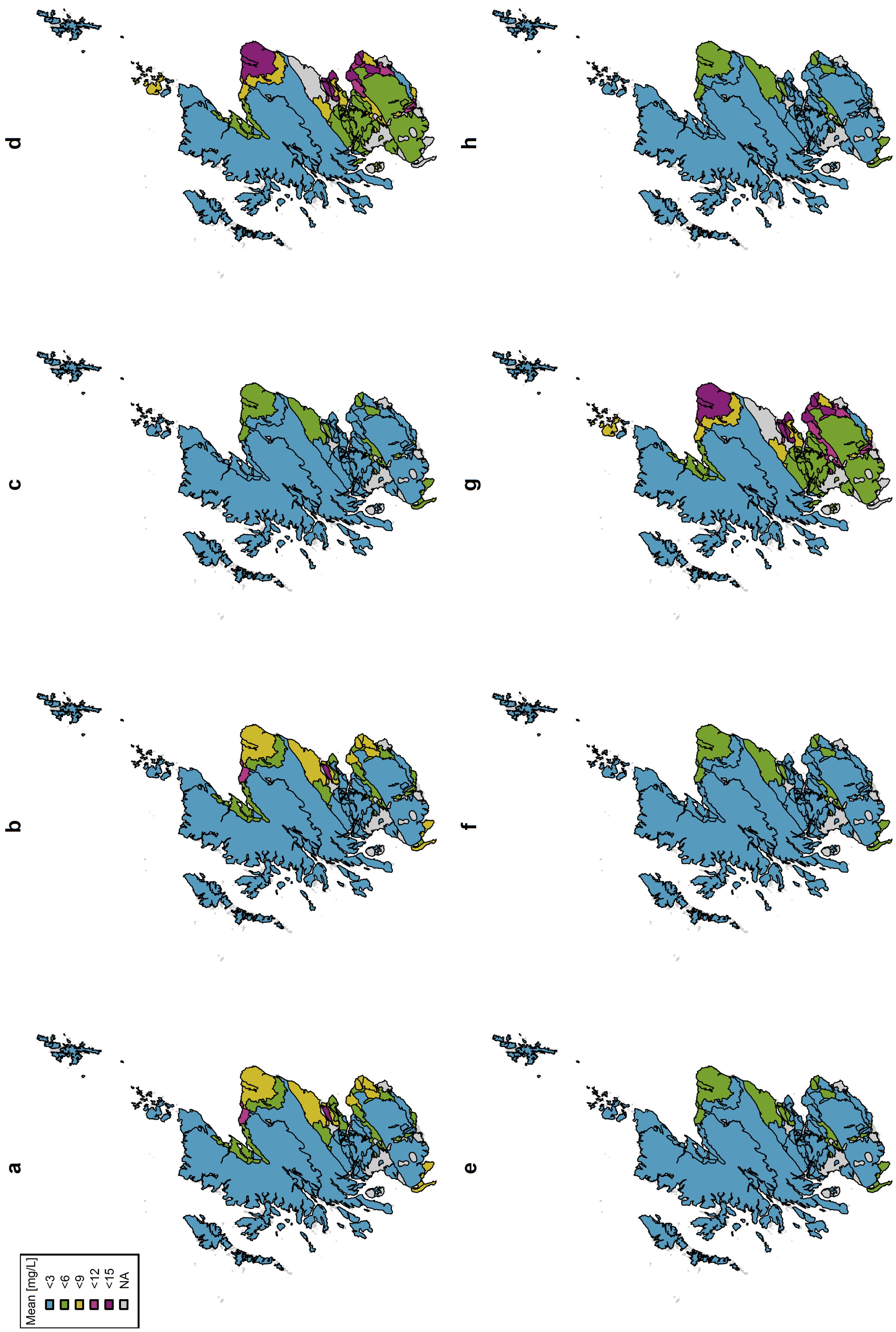

FIG. 6: Mean nitrate concentration in each ground water body group, as predicted by the emulator, under each of the modified climate scenarios. Labelling of the scenarios is as given in the list at the start of Appendix B.

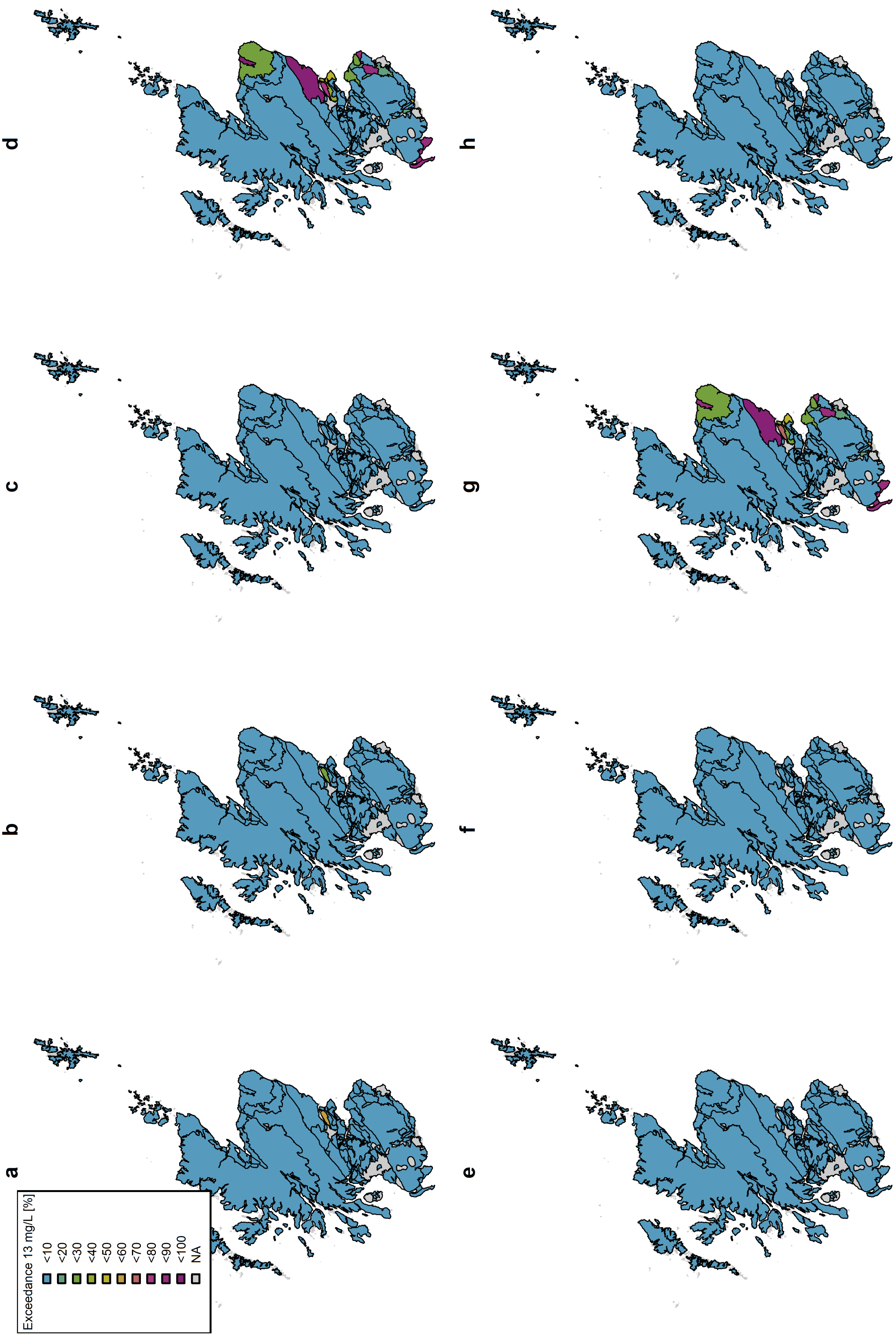

FIG. 7: Probability that the average nitrate concentration within each of the ground water body groups exceeds a threshold of 13 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix B.

FIG. 8: Probability that the average nitrate concentration within each of the ground water body groups exceeds a threshold of 37 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix B.

FIG. 9: Probability that the average nitrate concentration within each of the ground water body groups exceeds a threshold of 50 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix B.

FIG. 10: Probability that the nitrate concentration in at least one cell within a given ground water body group exceeds a threshold of 13 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix B.

FIG. 11: Probability that the nitrate concentration in at least one cell within a given ground water body group exceeds a threshold of 37 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix B.

FIG. 12: Probability that the nitrate concentration in at least one cell within a given ground water body group exceeds a threshold of 50 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix B.

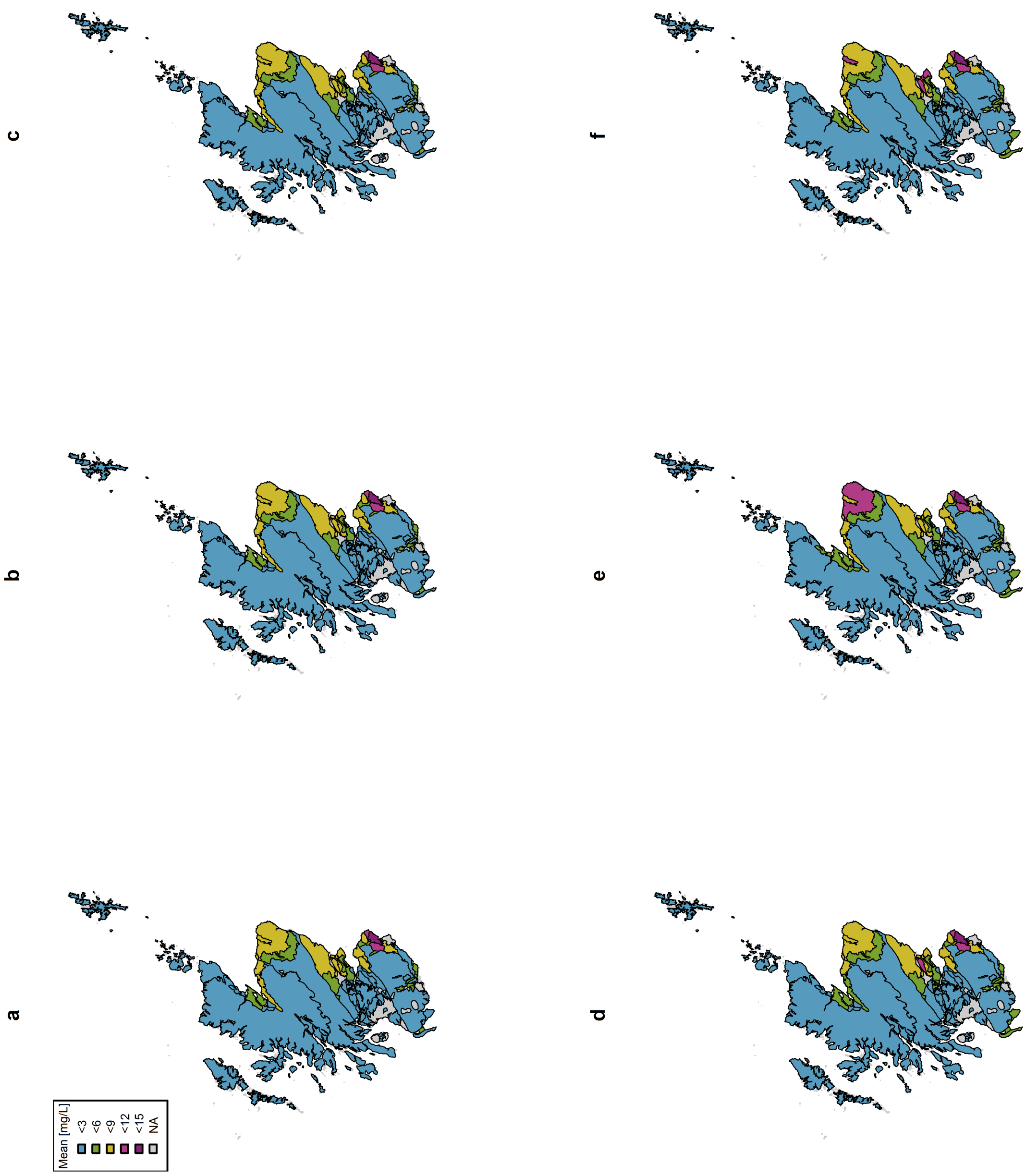

FIG. 13: Mean nitrate concentration in each ground water body group, as predicted by the emulator, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix B.

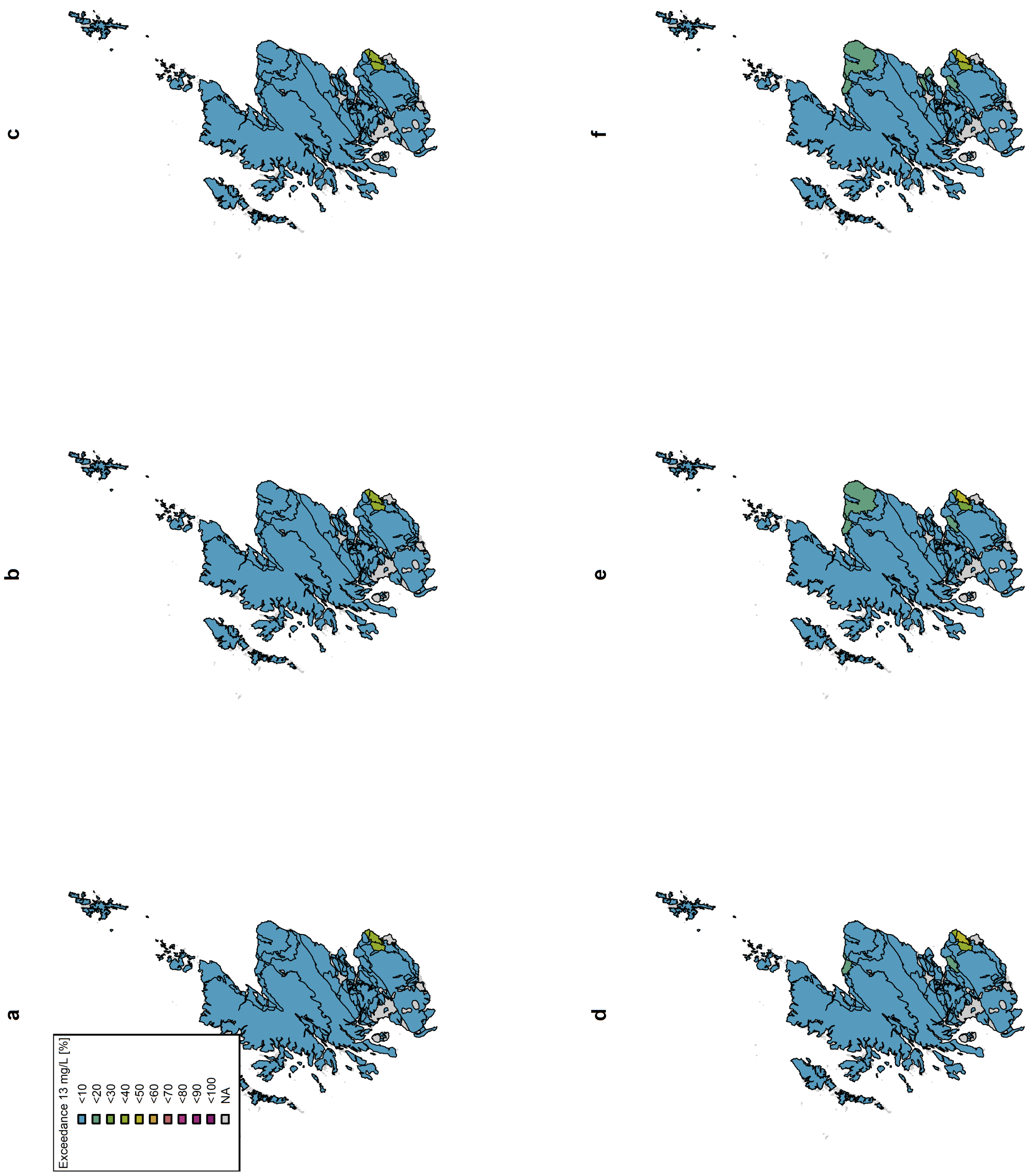

FIG. 14: Probability that the average nitrate concentration within each of the ground water body groups exceeds a threshold of 13 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix C.

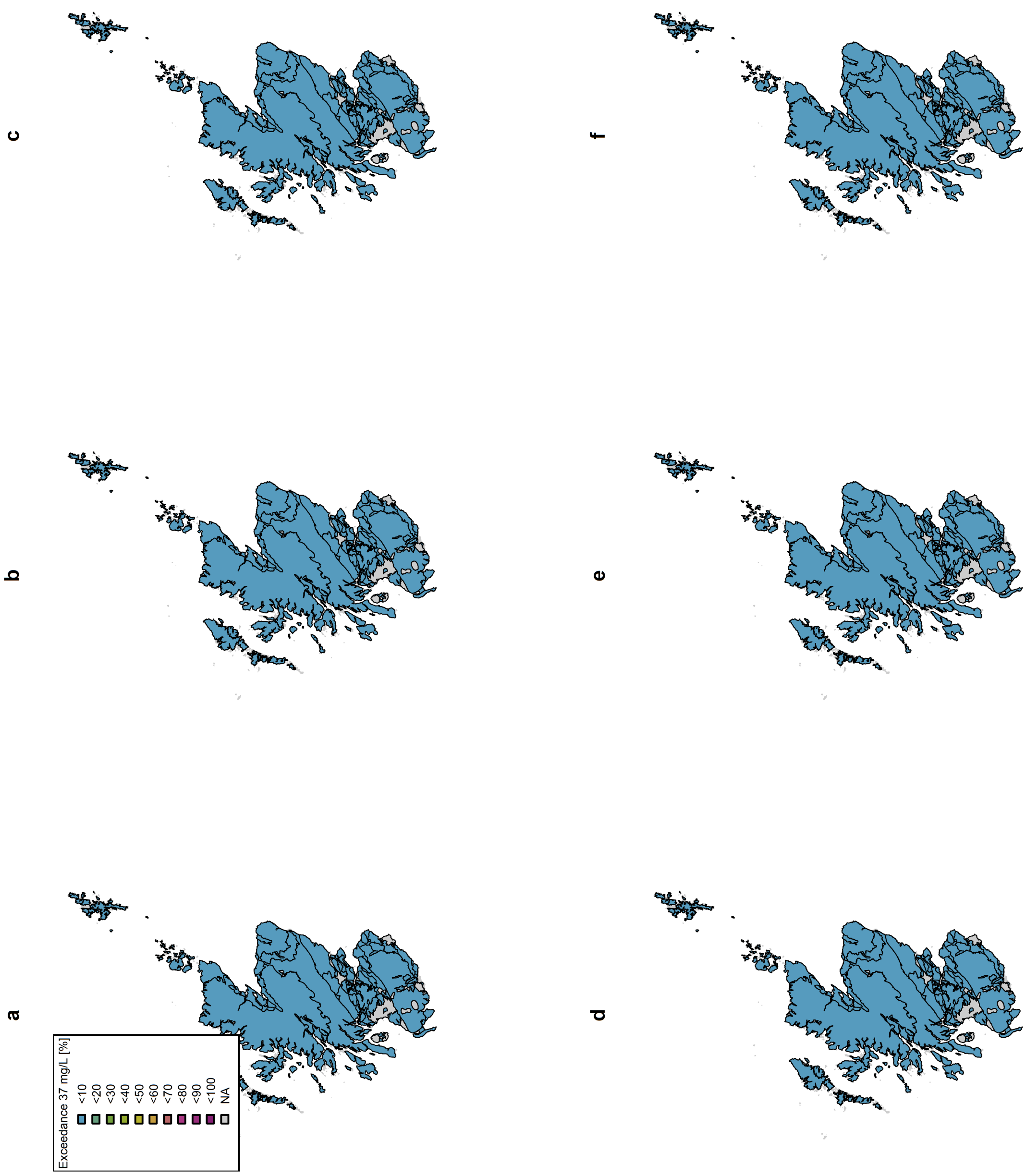

FIG. 15: Probability that the average nitrate concentration within each of the ground water body groups exceeds a threshold of 37 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix C.

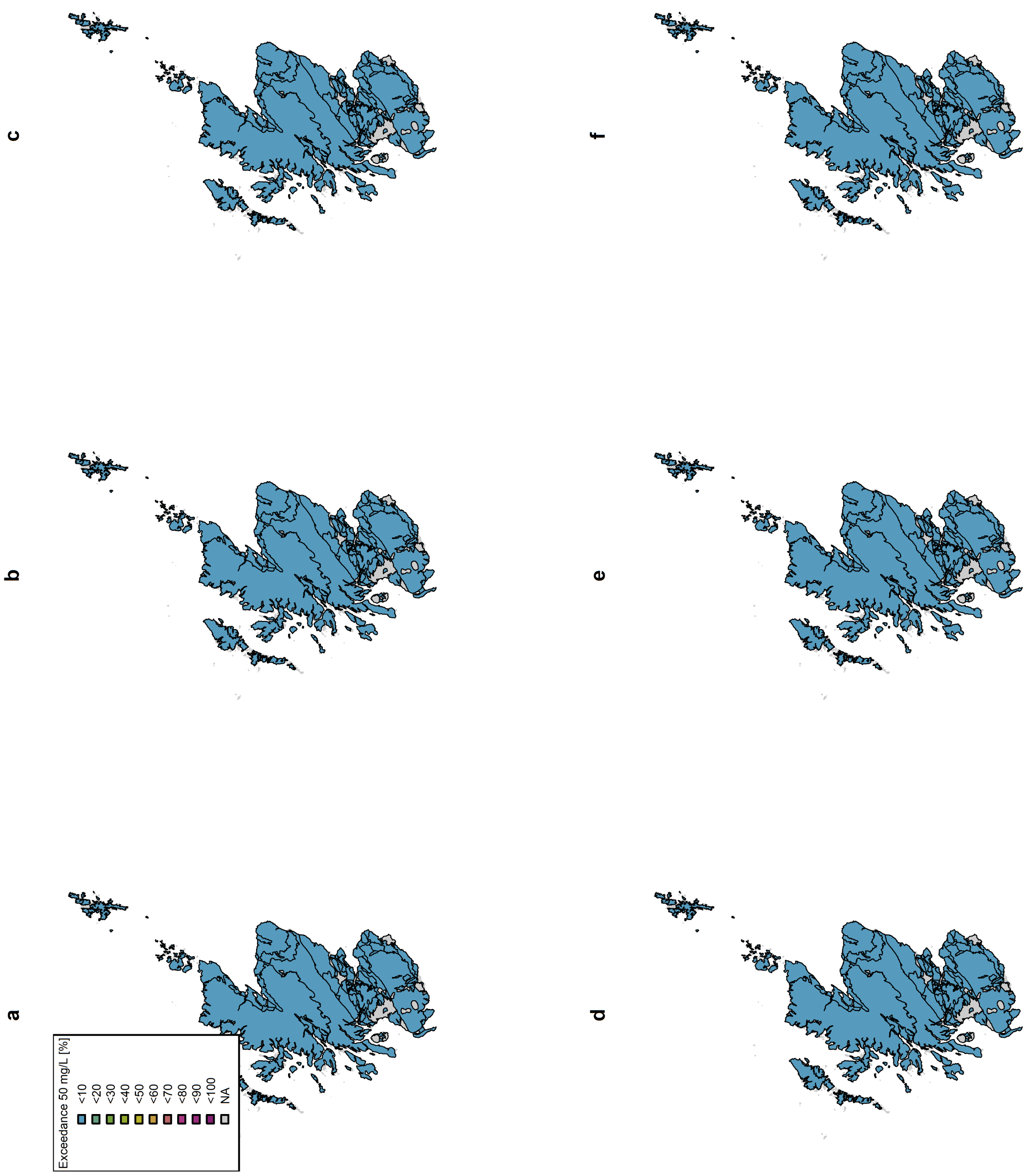

FIG. 16: Probability that the average nitrate concentration within each of the ground water body groups exceeds a threshold of 50 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix C.

FIG. 17: Probability that the nitrate concentration in at least one cell within a given ground water body group exceeds a threshold of 13 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix C.

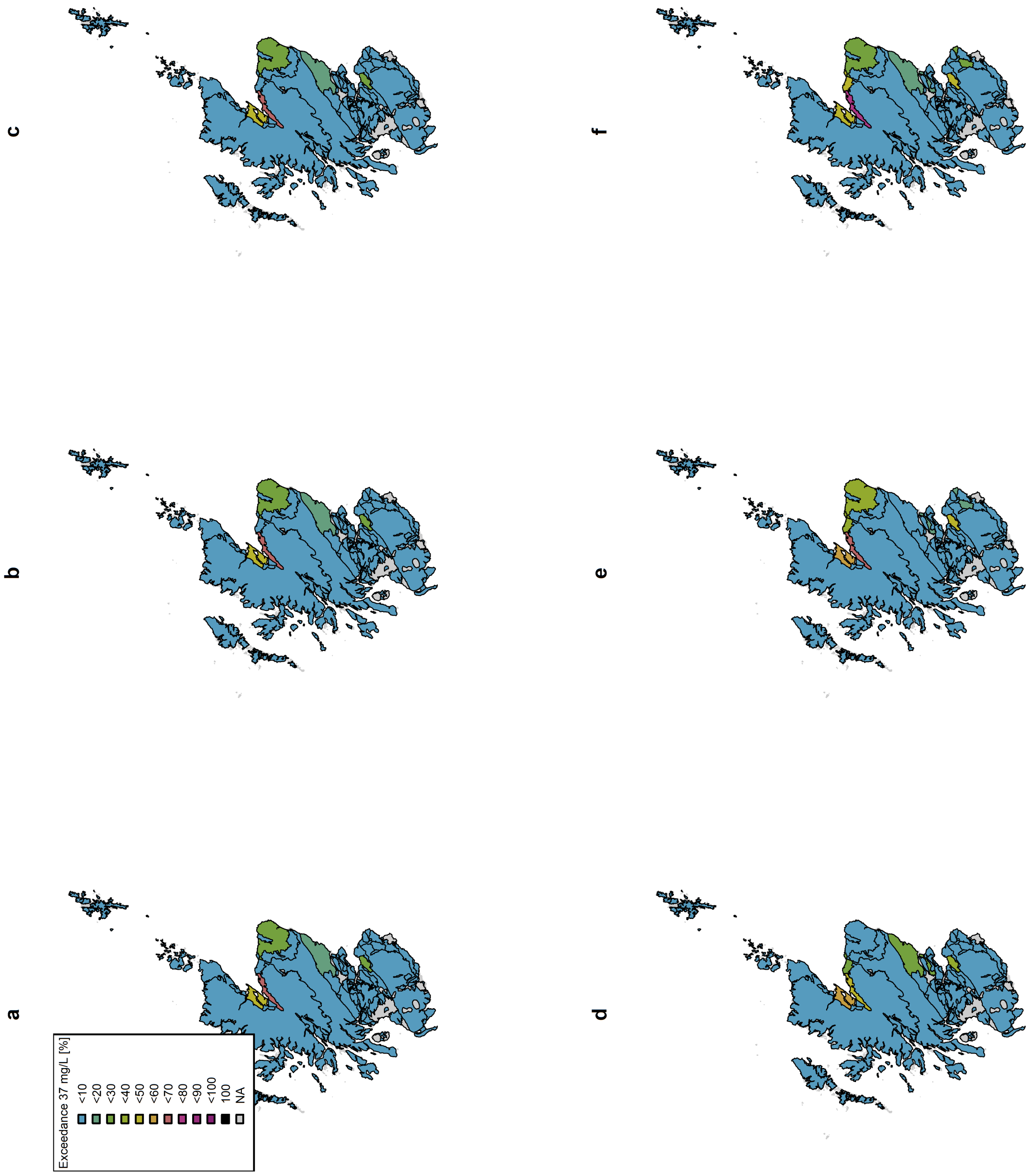

FIG. 18: Probability that the nitrate concentration in at least one cell within a given ground water body group exceeds a threshold of 37 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix C.

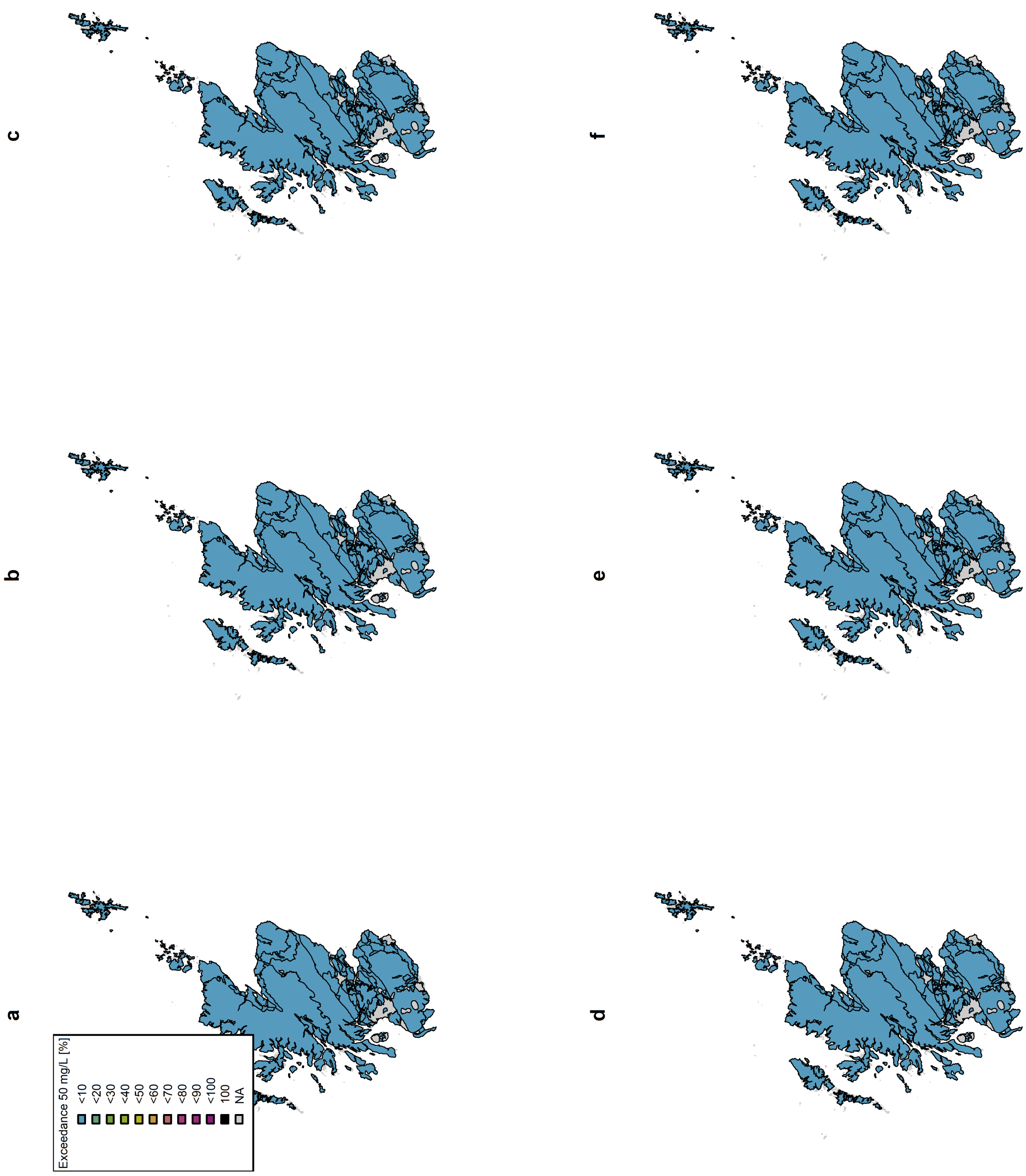

FIG. 19: Probability that the nitrate concentration in at least one cell within a given ground water body group exceeds a threshold of 50 mg/l, under each of the modified scenarios. Labelling of the scenarios is as given in the list at the start of Appendix C.