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Research Paper

Modelling spatial and inter-annual variations of nitrous oxide emissions from UK cropland and grasslands using DailyDayCent



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ABSTRACT

Agricultural soils are the primary source of nitrous oxide emissions due to management practices including fertiliser application. While fertiliser rates are one of the main drivers of nitrous oxide emissions, emissions are also dependent on other variables such as climate and soil properties. To understand the spatial and inter-annual variations in emission rate, simulations of N_2O emissions were made from 2000 to 2010 for UK grass and croplands. In addition, the sensitivity of these emissions to soil and climate inputs was also tested. Emissions of between 0.3 to 3.5 kg N ha⁻¹ yr⁻¹ and 0.7–7 kg N ha⁻¹ yr⁻¹ were simulated across UK croplands and grasslands, respectively. While inter-annual variations can be attributed to climate influences, the primary driver of spatial variations in emissions was soil clay content. However, when the sensitivity of nitrous oxide emissions to soil clay content alone was tested, it was not always the best predictor of emissions, when soil texture is altered outside of the normal range used as inputs to the model from different databases.

1. Introduction

National Greenhouse Gas inventories for quantifying emissions from agriculture and land use change often calculate emissions using default emission factors (EFs) coupled with country specific activity data in the form of land use and management information (IPCC, 2006; Ogle et al., 2013, 2014). To reduce uncertainty, and calculate estimates on a Tier 2 or 3 level, spatially disaggregated land use and land management information, in combination with country specific EFs, are increasingly being used. While the Intergovernmental Panel on Climate Change (IPCC) has proposed default EFs, they tend not to reflect local variations in climate and management (Skiba et al., 2012) and there is often not enough long term information to derive these EFs at regional level. Therefore, country specific EFs should be derived through experimental work, which in turn aims to reflect a degree of heterogeneity across the country of interest (Ogle et al., 2013) and also reflect a range of management practices (Bell et al., 2016). However, data from experimental

studies are understandably limited, both temporally and spatially, due to the resources required to conduct such experiments, and uncertainties still remain at a site level due to the spatial variability of soil properties (particularly nitrogen (N), carbon (C) and soil wetness). Therefore, simply extrapolating site derived EFs to a regional or national scale may not accurately reflect the complex interaction between soil, management, climate and crop type (Butterbach-Bahl et al., 2013).

More recently, biogeochemical models such as DailyDayCent (DDC; Parton et al., 1998; Del Grosso et al., 2008), DNDC (Frolking et al., 1998) and a number of other models (see Brilli et al., 2017 for a recent review), have been increasingly used to help fill these data gaps, as once calibrated, they allow for multi-annual simulations, and for users to test the effects of changing land management on emissions. Modelled assessments of emissions on a large spatial scale are uncertain due to uncertainties in inputs over large spatial scales, and inhenent uncertainty in model parameters (Gottschalk et al., 2007; Hastings et al., 2010; Fitton et al., 2014a,b). For example, some of the processes

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governing soil nitrous oxide (N_2O) emissions, outside of the effect of fertilisation, are poorly understood, and this is reflected in current biogeochemical models (Blagodatsky and Smith, 2012). In addition, spatial information on the different inputs required to simulate emissions, such as soil characteristics and management tend to be gathered at varying spatial resolutions and frequencies (Ogle et al., 2014), which is a particular problem when the aim of the modelling approach is inventory compilation. Therefore, in order to reduce uncertainties in simulated emissions model selection is of particular importance.

DailyDaycent is daily time step version of the Century model (Parton et al., 1998). Details of the processes that govern how DD works are detailed in Parton et al. (1998). In general DDC allows for users to simulate C and N dynamics from a range of different agricultural ecosystems. The model structure, while reasonably complex, allows for a good degree of flexibility in how different management scenarios can be implemented and does not require excessive input data in order for site level simulations to be implemented. Furthermore the efficacy of the model has been successfully tested on both crop and grassland sites across a range of countries including Canada, Germany, USA, Italy and Australia (Del Grosso et al., 2002; Abdalla et al., 2010; Scheer et al., 2014; Sansoulet et al., 2014). While in the USA the model has also been used to supply estimates for the national GHG inventory (Del Grosso et al., 2010) and is explored here to assess its potential for a similar role in the UK.

This study uses the DDC model to examine the annual and spatial variation in $\rm N_2O$ emissions from non – grazed UK grasslands and croplands for the years 2001 to 2010. While for both, management practices can be complex and alter the rate of emissions, the principal aim of this study is to improve understanding of the roles that soil, climate and N fertiliser application rates have on annual emissions, both for the UK as a whole and for the regions making up the UK including Scotland, Wales, Northern Ireland and England, which as the largest land area being re-divided into regional units. To this ends, simplified management was used, in combination with current national soil and climate grids to produce spatial $\rm N_2O$ emissions. Finally, the sensitivity of emissions to uncertainties in the model inputs; soil, climate and N application rates, was examined using Monte Carlo simulations to quantify the uncertainty and contribution of these inputs to uncertainty associated with simulated emissions.

2. Materials and methods

2.1. The DailyDayCent (DDC) spatial framework

2.1.1. DDC modelling approach

The initial calibration of the DDC model to site experimental data is described in Fitton et al. (2014a,b). Here experimental data from both experimental crop and grass sites located across the UK were gathered and the model was applied to each of the sites. However, rather than calibrating the model specifically for each site, a generic calibration approach was used, which avoided over fitting to the data. DDC was equally successful in simulating daily and annual N2O emissions from all sites (Fitton et al., 2014a,b). When simulating emissions from different grids or points across the UK, all site level input information is required, which includes information on crop and grass production, growth implementation (growing degree days versus dynamic carbon (C) allocation), water movement (Richards' or capacity approach) and the initialisation of soil C turnover *via* a long term spin up phase. As this information is not available for every location in the UK, values derived from the final site level simulations after the generic calibration (Fitton et al., 2014a,b), were used for the spatial simulations, and were not modified between the different grid cells.

2.1.2. Soil, climate and land input information

Initially, UK wide maps that contain the relevant information on land use (grass or crop), soil and climate were joined in ArcGIS to create

a national grid, at the finest resolution possible, which linked information on each input via a unique ID based on location. To populate the soil information required to run DDC for the relevant land use, input data was obtained from the Harmonised World Soil Database (HWSD). The HWSD provides separate soil pH, bulk density, sand, silt and clay contents for soils that would be classified as existing under grassland or croplands. This information was supplied on a 1 km² grid and for up to 10 soil series in each grid up to a depth of 1 m. In addition, since the HWSD database has information at the finest resolution of all datasets used in this study, it was used as the resolution of the outputs. Climate information was sourced from the Meteorological Office Rainfall and Evaporation Calculation System (MORECS, Hough and Jones, 1998) grid. This database, which is on a 5 km² grid provides the daily climate information (temperature: maximum and minimum and precipitation) from 1961 to 2010 required to drive DDC. While other climate inputs were available from this database, only the temperature and precipitation data were used, in line with the available information from the generic calibration.

The land management component, which is governed in DDC via schedule files, also required to run DDC (Del Grosso et al., 2008), are more complicated to create, as the schedule file requires management event types and their dates to be detailed on an annual basis. Due to their complexity, for grasslands, a simplified approach was followed, whereby across the UK, no grazing occurred and the swards were harvested three times during the growing season May, (June/July) and also October. For uniformity across the UK, fertiliser was applied in the form of ammonium nitrate (AN) at a rate of 80 kg N ha⁻¹ yr⁻¹. This value was selected since over the last couple of decades, fertiliser application rates on both grass and croplands have steadily declined and specifically for the period of interest for this study, N application rates on UK grasslands have declined from 99 to 63 kg N ha⁻¹ yr⁻¹ (BSFP, 2015). A rate of 80 kgN ha^{-1} yr⁻¹ therefore roughly reflects the UK average rate of N applied in the UK between 2000 and 2010 (BSFP, 2015). Throughout the UK, fertiliser was applied between April and July, three times in equal splits, and the only adjustment made regionally was the date of the first application of AN only. More specifically, in MORECS squares with an average winter temperature < 5 °C, the first fertiliser application was delayed by 10 days. In MORECS squares with an average temperature of > 6 °C, the first fertiliser application was brought forward by 10 days, and finally for those with temperature between 5 °C and 6 °C, fertiliser application occurred on the 10th April, before the first harvest.

For croplands, the UK was subdivided into smaller regional units consisting of Wales, Scotland, Northern Ireland and England; which were subdivided further into 11 smaller regional units. The annual crop to be sown and rotational sequence for the period 2001 to 2010 for each region was generated by following Holman et al. (2005). Crop rotation data was not available for Scotland and Northern Ireland, so both regions were assigned the same crop rotation as northern England. Fertiliser rates were pre-set, for cereal crops at 140 kg N ha $^{-1}$ yr $^{-1}$ and for oilseed rape at 60 kg N ha $^{-1}$ yr $^{-1}$, and fertiliser was applied two or three times during the year in equal splits depending on the crop. Here, as with grasslands, fertiliser was applied in the form of ammonium nitrate and the application rates were selected based on information in the British survey of fertiliser practice (BSFP, 2015). Sowing, harvest N application dates, were regionally adjusted based on information provided within the MORECS grid, as described previously.

As part of the process of calibration of the DDC model (Fitton et al., 2014a,b), long term history of the site or grid of interest was written into the scheduling file to allow for an establishment of the soil organic matter (SOM) pool sizes, and also establishment water movement through the soil profile. As this information is not available across the UK, the same long term management was used to initiate the DDC spin up as used in the generic calibration (Fitton et al., 2014a,b). More specifically, it was assumed that from 1500 onwards there was forest planted, this was then removed and converted to grasslands, which

from 1900 to 1950 had little or no management. For then until the period of interest, each site was managed with low N inputs until conversion to the current land management. Finally, for each grid identified by joining the soil and climate database, a corresponding schedule file was created containing the management information for the land use and region of interest.

2.1.3. Spatial framework of DDC

To run the spatial simulations, an automated framework retrieved the soil, climate and schedule file for each unique $1~\rm km^2$ grid. The relevant soil and climate information for each grid was then extracted for each grid and converted into the format required by DDC. Depending on the land use, the corresponding schedule file was then written to drive the management of the grid cell of interest, and a software wrapper was created, in R, to allow the DDC executable file to be run automatically for each grid cell. Finally, outputs of annual and crop yields were calculated and the results of the spatial run were written to separate output text files. This step was repeated for each of the 10 soil series, for both land uses, defined by the HWSD soils database.

3. Sensitivity, uncertainty simulations and statistical analysis

The information contained within spatial databases, tend to be ground truthed observations scaled upwards. Therefore within both the soil and climate databases for each 1 km and 5 km grid respectively, there is uncertainty in the values selected to represent the grid. In addition, as within the study a fixed N application rate was used, an analysis of the sensitivity of simulated N_2O emissions to changes in these inputs across the UK was undertaken. To do this, a similar approach to those adopted in Hastings et al. (2010) and Fitton et al. (2014a,b) was adopted. However, both of those studies focused on site level uncertainty, and changes at each site simulated were based on a fixed percentage change in each input variable based on an expert survey conducted within the Hastings et al. study. Here, the actual range of values across all 1 km² grid within each of the 11 UK regions of each input, which occurred within the two most dominant soil series, was used to define the range of uncertainty, as described below.

For all of 1 km² grids occurring within a region defined as grass or cropland, the standard deviation (SD) in the range of values for soil pH, bulk density and clay content was extracted. This in turn, was then deemed to be the uncertainty range around each input for each of the 1 km² grids, within that region. Due to its importance for N_2O emissions, the sensitivity of annual emissions to changes in N application rates was also tested. Here, it was assumed that the rate of N application could vary by $+/-\,$ 10%.

For temperature and precipitation, the standard deviation in daily

values was first calculated and then the average SD in daily values was used as the range of uncertainty to be applied to daily values. For the sensitivity analysis, 10 equal interval step changes in each input were simulated. The maximum and minimum values simulated for each input in each grid was the input's original grid value ± one standard deviation value for the region. For each input change, all other input variables were held at their original value. For the fertiliser application rates, the maximum and minimum values were the original value ± 10% of the total annual N applied. This arbitrary value was selected, because unlike soil inputs, there was no information on the uncertainty around N application rates. In addition, this focuses on the response of emissions to changes in inputs rather than absolute change. Since fertiliser rates tend to have a strong linear influence on the rate of emissions, increasing the range of values simulated when management for each gird was the same, could potentially mask the role of other inputs. For reasons of computational efficiency, a sub sample of the 1 km² grid cells within each region were randomly selected for use in the sensitivity and Monte Carlo analysis. For the two most dominant soil series, which tend to account for between 70 and 90% of the entire 1 km² grid, all grids were deemed to have equal weight and $75 \times 1 \text{ km}^2$ grids,

within each region, were randomly selected for the dominant soil series, and for the second most dominant soil series, $50 \times 1 \, \mathrm{km}^2$ grids were randomly selected. To test the interaction uncertainty between different inputs on the rate of annual emissions, for each region, the 10 inputs available for each input parameter were assumed to have had equal weight, and were assumed not co-vary, so that each input could be repeatedly re-sampled independently. Seventy five combinations of each of these inputs were then randomly sampled for the Monte Carlo simulations. For each region and the 75 subsample $1 \, \mathrm{km}^2$ grids, the sensitivity simulations (10 step change for each individual input) were simulated, followed by 75 combinations of inputs.

Once completed, for both land uses, a Pearson correlation analysis was undertaken (using Minitab $^{\circ}$) between the long term average annual emissions of N_2O and the input parameters. Here, for each $1~\rm km^2$ grid under each land use, the 10 year average annual N_2O emissions were aligned with their corresponding soil; pH, bulk density and clay content and the average annual temperature and annual precipitation. In addition, a simple linear regression between the datasets was also carried out in Minitab. Both of these tests were initially performed on all grids across the UK and the analysis was then repeated again on a regional level, to examine any regional differences. Because croplands are subject to rotation, simulated crop yield was included as an additional variable.

Finally, to test the sensitivity of the modelled N_2O emissions to changes in soil, climate and fertiliser inputs, the contribution of each input, via the contribution index, to total uncertainty was calculated using the formula outlined in Vose (2000), Gottschalk et al. (2007) and Fitton et al. (2014a,b):

$$c_i(contribution\ index) \frac{\sigma_g - \sigma_i}{\sum_{i=1}^{i_{max}}\ (\sigma_g - \sigma_i)} \times 100$$

Where c_i is the contribution index (%) in factor i, σ_g is the standard deviation in the total uncertainty, calculated across the long term average annual N₂O emissions simulated via the Monte Carlo simulations, σ_i is the standard deviation of the range of values simulated as part of the sensitivity analysis of each input, i, where i is the specific input of interest at the time, and i_{max} is the total number of model input factors considered. The contribution index was calculated for separately for each region and the grass or croplands simulated.

4. Results

4.1. Spatial N2O emissions from UK grass and croplands

The average annual N_2O emissions from the two dominant soil types defined as occurring on UK grassland and croplands from 2001 to 2010 are detailed in Figs. 1 and 2, respectively.

For UK grasslands, the range of simulated annual emissions was large and varied from 0.5 to 7 kg $N_2O\,-\,N\,ha^{-1}\,yr^{-1},$ tending to fall within the range of expected emissions reported in measured data reported in UK based experimental and modelling studies (Fitton et al., 2014a,b; Chadwick et al., 2014; Bell et al., 2015a,b). The highest emission rates tended to occur in north-west Scotland, where higher soil C and a relatively wetter climate are found, compared to other regions of the UK. As grassland management was assumed to be the same across the UK, while N fertiliser was a driver of emissions, the results demonstrated how N2O emissions varied in relation to soil and climate drivers. For all grids across England, long term (10 year) averages in annual N2O emissions from grasslands were most correlated with changes in clay content, bulk density and precipitation, though each had different effects on emissions. For England as a whole, soil pH and temperature tended to show a positive correlation with the rate of emissions (Table 1). However in each case, the relationship between these was not as well defined as for clay content. However, when the same analysis for bulk density was repeated for a sample of some of the

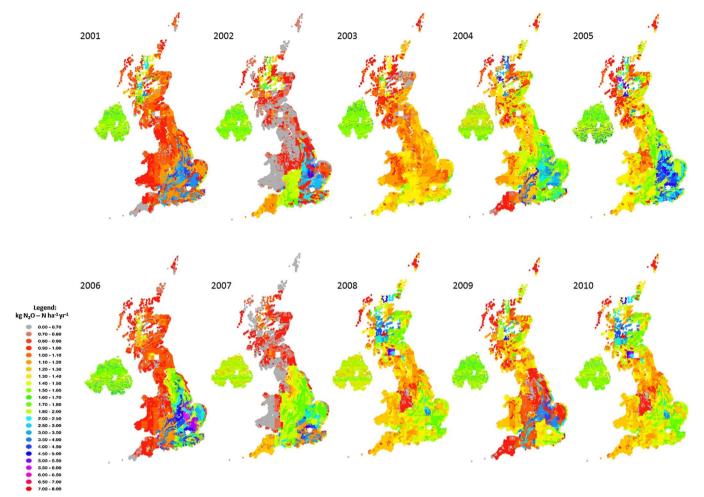


Fig. 1. Annual N_2O emissions for grasslands for the years a) 2001, b) 2002, c) 2003, d) 2004, e) 2005, f) 2006, g) 2007, h) 2008, i) 2009 j) 2010.

smaller regions within England, the correlation coefficient between $\rm N_2O$ and the inputs varied. Similarly for the clay content, regionally, the contribution of clay content varied depending on the region tested, explaining between 38 and 90% of the variation in $\rm N_2O$ emissions. In addition, regardless of the actual contribution on a regional basis, clay content tended to be the best predictor of annual emissions, when averaged over a 10 year period. The exception to this was in Scotland where clay content and bulk density, on their own, were equally good predictors of $\rm N_2O$ emissions. The effect of the remaining soil and climate inputs varied by region, while in general, each of the values tended to be poorer predictors, especially when compared with clay content, though bulk density was often the second best predictor.

Modelled emissions of N2O from croplands (2001-2010) ranged from 0.3 to $3.5 \text{ kg N}_2\text{O} - \text{N ha}^{-1} \text{ yr}^{-1}$ (Fig. 2). Crop yields varied between 0 and 10 t DM ha⁻¹ and simulated values depended on the type of crop that was sown in the year of interest (Fig. 3). It is important to note that as part of the crop rotation sequence used in this study the cropland was left fallow after the harvesting of, for example, oil seed rape late in year 1 until the planting of, for example, winter wheat in year 2. As winter wheat is not harvested until year 3, year 2 harvests were selected to be 0 kg N ha⁻¹ yr⁻¹ to reflect that no crop yield was taken that year. Much like grasslands, nationally, the highest rate of N2O emissions tended to occur in Scotland. However, since crop rotation, and hence the amount of N applied with the crop was different, inter-annual and spatial variations of annual N2O emissions varied significantly with crop type and hence yields, so yield was also included as a predictor for annual emissions (Table 2). Clay content accounted for most of the variation in long term average annual emissions. This was true regardless of the region studied, and across the selected regions, clay content was also the best predictor for estimating long term emissions from croplands. While other soil parameters accounted for some variation, crop yields also accounted for a significant proportion of the variation in emissions, though the contribution varied regionally (Table 2). For Scotland there was a particular difficulty in attributing patterns of emissions due to spatial variations in the different inputs, and subsequently using these as predictors for changes in emissions. For example, for croplands in the different regions of England, Wales and N. Ireland, the correlation coefficient between clay content and $\rm N_2O$ emissions ranged from 0.62 to 0.95, whereas in Scotland this value was 0.34.

4.2. Sensitivity and Monte Carlo simulations

The regional variation in each input parameter used as part of both the sensitivity and Monte Carlo simulations are detailed in Table 3. Here, for ease of presentation, values represent a sample of some of the regions within the UK, and also the maximum change (increase or decrease), from the input parameters original value. For both grass and croplands, an arbitrary +/-10% change in the rate of N was applied across the UK regardless of the initial N rate and the region of interest. The impact of changing each input parameter on the average annual emissions of the sampled sites, from the two most dominant soil series from crop and grasslands across the UK, are detailed in Table 4. Values represent the percentage change in long term annual emissions, compared to those calculated using the original inputs from the sampled sites, termed the baseline emissions. Across England's grasslands,

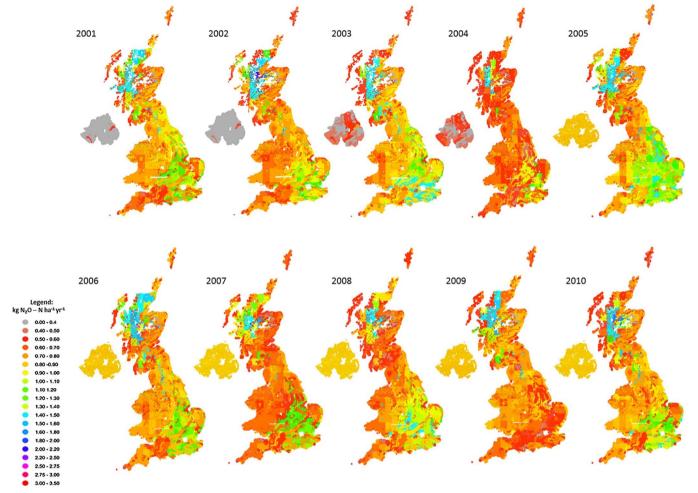


Fig. 2. Annual N2O emissions for cropland for the years a) 2001, b) 2002, c) 2003, d) 2004, e) 2005, f) 2006, g) 2007, h) 2008, i) 2009 j) 2010.

changes in the average annual precipitation values led to the greatest difference from baseline emissions, which, in turn, varied by region (Table 5). This may be because precipitation change is simulated as a daily modification, and it more directly affects soil water filled pore space, and hence the daily pattern of N₂O emissions (Fitton et al., 2014b). While changes in the remaining inputs can also affect the rate of emissions, these changes tend not to alter the baseline trends in daily emissions, and only alter the magnitude. Of these, N₂O emissions also tended to be sensitive to changes in the rate of fertiliser N application, where increasing or decreasing N rates led to corresponding increases or decreases in N₂O emissions. In addition, both on larger spatial scales e.g. England, and for the smaller regional units, e.g. Anglia, while changing N applications did not always lead to the same percentage

change in emissions, N_2O emissions exhibited a linear response to changes in N rates, so N rate is a good predictor for understanding the range of emissions within a region. However, it is important to note this relationship was calculated based on a limited range of N application rates, and does not account for variations in N emissions due to changing application dates.

The contribution of each of the inputs to uncertainty in the average annual emissions from the selected 1 km grid cells, produced from the Monte Carlo simulations of grassland sites, showed that for each region, uncertainty in the fertiliser application rate tended to account for between 12% and 18% of the total uncertainty (Fig. 4). However, this is constrained by the relatively small change in N application rates. For the remaining inputs, the regional difference varied significantly. For

Table 1
Pearson correlation analysis and single regression for the spatial variation of the 10 year average annual emissions for grasslands from selected regions in the UK.

| Pearson correlation coefficie | ent | | Regression analysis (R ²) | | | | | | | |
|-------------------------------|-------|--------------|---------------------------------------|-------------|---------------|------|--------------|---------|-------------|---------------|
| Region | Clay | Bulk density | Soil pH | Temperature | Precipitation | Clay | Bulk density | Soil pH | Temperature | Precipitation |
| England | 0.85* | -0.27* | -0.06* | 0.15* | -0.3* | 0.73 | 0.1 | 0.002 | 0.02 | 0.10 |
| Anglia – England | 0.86* | -0.28* | -0.63* | 0.37 | -0.21* | 0.39 | 0.1 | 0.007 | 0.28 | 0.28 |
| East midlands - England | 0.55* | -0.31* | -0.09* | 0.53* | -0.53* | 0.66 | 0.1 | 0.021 | 0.05 | 0.004 |
| Wessex - England | 0.81* | -0.13* | -0.15* | -0.21* | -0.06* | 0.65 | 0.32 | 0.005 | 0.003 | 0.009 |
| South east - England | 0.97* | -0.65* | -0.28* | -0.05* | -0.07* | 0.95 | 0.42 | 0.08 | 0.0005 | 0.004 |
| Scotland | 0.37* | 0.34* | 0.06* | -0.16* | 0.17* | 0.35 | 0.35 | 0.1 | 0.15 | 0.18 |
| Northern Ireland | 0.94* | -0.48* | 0.40* | 0.13* | 0.1* | 0.88 | 0.23 | 0.14 | 0.02 | 0.01 |
| Wales | 0.72* | 0.05* | 0.27* | 0.16* | -0.41* | 0.52 | 0.1 | 0.1 | 0.03 | 0.2 |

^{*}Indicates a p values < 0.001.

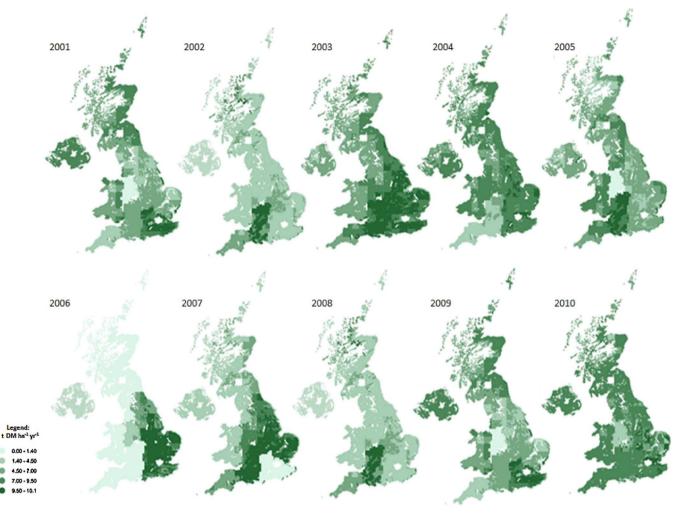


Fig. 3. Annual crop yields for croplands for the years a) 2001, b) 2002, c) 2003, d) 2004, e) 2005, f) 2006, g) 2007, h) 2008, i) 2009 j) 2010.

Wales and Northern Ireland, temperature accounted for 48% and 45% of the total uncertainty, respectively, which is not unexpected since both have slightly colder climates, especially in the summer, when compared to southern England. For England, while temperature accounted for only 7% of the uncertainty around the emissions, there was an almost equal split in the contribution of each input to uncertainty; this is primarily because the larger land mass of England includes a wider range of soil and climate types. Despite this, clay content, regardless of region, always accounted for more than 20% of the total uncertainty, indicating its importance in estimating annual emissions (Fig. 4).

For the sampled cropland sites, the range in the percentage change

of annual emissions due to changes in each of the inputs (Table 4), was smaller than those of grasslands. Any change in bulk density or clay content tended to lead to an increase in emissions compared to the baseline, for each of the regions within the UK. It is important to note that when tested on a large spatial scale such as England, because each region can have a different crop rotation sequence and different management, it is difficult to detect different sensitivities of average annual emissions to changes in the soil and climate inputs. As with grasslands, for the different regions, the response of emissions could be more accurately detected, and as for grasslands, differed by region. The efficacy of most of these inputs as a predictor of the sensitivity of emissions within a region varies, but unlike for grasslands, clay content could be

Table 2
Pearson correlation analysis and single regression for the spatial variation of the 10 year average annual emissions from croplands for selected regions in the UK.

| Pearson correlation coeffici | Regression analysis (R ²) | | | | | | | | | | | |
|------------------------------|---------------------------------------|--------------|---------|-------------|---------------|-------|------|--------------|---------|-------------|---------------|-------|
| Region | Clay | Bulk density | Soil pH | Temperature | Precipitation | Yield | Clay | Bulk density | Soil pH | Temperature | Precipitation | Yield |
| England | 0.9* | -0.17* | 0.08* | 0.36* | -0.48* | 0.62* | 0.79 | 0.03 | 0.006 | 0.1 | 0.23 | 0.39 |
| Anglia – England | 0.95* | -0.16* | -0.58* | 0.25* | 0.39* | 0.59* | 0.9 | 0.03 | 0.34 | 0.06 | 0.15 | 0.35 |
| East midlands - England | 0.95* | -0.44* | -0.27* | 0.47* | -0.43* | 0.75* | 0.9 | 0.19 | 0.07 | 0.22 | 0.19 | 0.57 |
| Wessex – England | 0.93* | -0.11* | -0.004* | -0.005* | -0.16* | 0.85* | 0.89 | 0.012 | 0.018 | 0.002 | 0.02 | 0.72 |
| South east - England | 0.95* | -0.6* | 0.29* | 0.05* | -0.15* | 0.16* | 0.68 | 0.02 | 0.1 | 0.19 | 0.22 | 0.54 |
| Scotland | 0.34* | -0.05* | 0.47* | -0.1* | -0.03* | 0.2* | 0.12 | 0.002 | 0.22 | 0.1 | 0.01 | 0.4 |
| Northern Ireland | 0.62* | 0.04* | 0.76* | 0.25* | 0.07* | 0.41* | 0.38 | 0.002 | 0.62 | 0.1 | 0.01 | 0.2 |
| Wales | 0.71* | 0.38* | 0.64* | 0.34* | 0.40* | 0.46* | 0.51 | 0.14 | 0.41 | 0.42 | 0.11 | 0.16 |

^{*}Indicates a p values < 0.001.

Table 3The standard deviation in the range of values of each input parameter of each of the regions in the UK for the two most dominant soil series.

| Grasslands | | | | | Croplands | | | | | | |
|----------------------------|----------|--------------------------------------|---------|------------------|--------------------|----------|--------------------------------------|---------|------------------|-----------------------|--|
| Region | Clay (%) | Bulk density (gcm ⁻³) | Soil pH | Temperature (°C) | Precipitation (mm) | Clay (%) | Bulk density (gcm ⁻³) | Soil pH | Temperature (°C) | Precipitation (mm) | |
| Anglia – England | 16.8 | 0.22 | 0.45 | 0.56* | 0.09* | 16.8 | 0.22 | 0.45 | 0.56 | 0.09 | |
| East Midlands – England | 17 | 0.14 | 0.7 | 0.7* | 0.13* | 17 | 0.11 | 0.71 | 0.7 | 0.13 | |
| North East – England | 9.3 | 0.21 | 0.74 | 0.99* | 0.22* | 9.9 | 0.14 | 0.77 | 0.99 | 0.22 | |
| North - England | 5.8 | 0.25 | 0.62 | 1.02* | 0.24* | 5.9 | 0.23 | 0.65 | 1.02 | 0.24 | |
| North Mercia – England | 5.9 | 0.14 | 0.66 | 0.75* | 0.14* | 5.2 | 0.15 | 0.64 | 0.75 | 0.14 | |
| South East – England | 16.3 | 0.11 | 0.74 | 0.75* | 0.13* | 15.8 | 0.11 | 0.68 | 0.75 | 0.13 | |
| South Mercia – England | 13.8 | 0.07 | 0.56 | 0.69* | 0.13* | 13.9 | 0.07 | 0.57 | 0.69 | 0.13 | |
| South West – England | 6.65 | 0.15 | 0.49 | 0.71* | 0.14* | 6.1 | 0.11 | 0.48 | 0.71 | 0.14 | |
| Wessex - England | 14.4 | 0.17 | 0.89 | 0.66* | 0.13* | 14.4 | 0.17 | 0.89 | 0.66 | 0.13 | |
| Scotland | 39 | 0.05 | 0.25 | 0.68* | 0.16* | 32 | 0.12 | 0.27 | 0.65 | 0.15 | |
| Northern Ireland | 38 | 0.14 | 0.34 | 0.68* | 0.17* | 9.2 | 0.33 | 0.57 | 0.52 | 0.12 | |
| Wales | 44 | 0.09 | 0.33 | 0.47* | 0.09* | 35 | 0.13 | 0.29 | 0.71 | 0.17 | |

^{*} Indicates a change in daily values.

used as a predictor in all regions (Table 5). Fertiliser application rate is the primary driver of uncertainty in N_2O emission estimates (Fig. 5, a). Since the calculations are based on inter-annual averages, and cropland fertiliser rates vary accordingly, fertiliser application rate accounted for between 56% and 62% of the uncertainty from the Monte Carlo simulations. For the remaining inputs, temperature and precipitation accounted for most of the variation in emissions, whereas for England, Scotland and Northern Ireland, temperature accounted for up to 18%, and in Wales, precipitation also accounted for 18% of the uncertainty in modelled N_2O emissions (Fig. 5,b).

5. Discussion

Building on previous site-level simulations detailed in Fitton et al. (2014a,b), this study aimed to provide an understanding of both the spatial an inter-annual variations in nitrous oxide emissions in the UK. To do this, a simplified representation of the management of UK

agricultural land was combined with spatial datasets of soil, climate and land use. This approach allows for an understanding of the role other drivers of N_2O emissions; soil and climate, potentially on the rate of emissions. In addition, this approach provides insight into how uncertainty in input parameters affects estimates of N_2O emissions.

For non–grazed grasslands, assuming the same management across the UK, we found that nitrous oxide emissions were most correlated with clay content. Across all the different regions of the UK, N_2O emissions increased with increasing clay content. This is consistent with a similar Canadian study, which found a 50% increase in emissions when moving from coarse to medium textured soils (Rochette et al., 2008). While clay content was also found to be the best single predictor of N_2O emissions, an element of caution must be applied when using clay content or soil texture in this manner. As seen in the sensitivity analysis, changing the clay content while holding the remaining inputs fixed did not result in a linear response. This may have been due to the range of values selected as part of the sensitivity and Monte Carlo

Table 4

Annual average emissions (N2O – N kg ha-1 yr-1) for the sampled sites in each region using original input values (baseline) and the percentage change in emissions when values are increased from initial input value (mean +'ve) or decreased from original input value (mean -'ve).

| Region a) Baseline Grasslands | Baseline | Bulk density (g cm ⁻³) | | Clay content (%) | | Soil pH | | Precipita | tion (mm) | Temperature (°C) | | Fertilisation rate (kg N ha ⁻¹ yr ⁻¹) | |
|----------------------------------|----------|------------------------------------|-------------|------------------|----------------|----------------|----------------|----------------|-------------|------------------|----------------|---|----------------|
| | | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) |
| England | 2.3 | -4.35 | -8.7 | -12.7 | -8 | -8 | -17 | 0 | 34 | 0 | 0 | 5.7 | -8.7 |
| Anglia | 1.96 | 5 | -5 | -7 | -16 | -25 | 13 | -2 | 28 | -2 | -2 | 6 | -7 |
| East midlands | 2.2 | 6 | -10 | -13 | -14 | -8 | 5 | 0 | 2 | 0 | 0 | 9 | -6 |
| Wessex | 2.8 | 30 | -12 | -19 | -22 | -32 | 16 | 0 | 0 | -3 | -3 | 7 | -8 |
| South east | 2.3 | 3 | -8 | -17 | -14 | -18 | -1 | 1 | 0 | -2 | -2 | 9 | -7 |
| Scotland | 1.2 | 8.3 | 0 | 1.7 | 0.8 | -11 | -8.3 | 0 | -6.7 | 2.5 | 3.3 | 2.5 | -4.2 |
| N. Ireland | 1.2 | 3.5 | 8.3 | 0 | 0.8 | -15 | -8.3 | 0 | -1.7 | 0.8 | 0.8 | 10 | -15.4 |
| Wales | 1.2 | 3.3 | 2.5 | 2.5 | 2.5 | -5.8 | -7.4 | 0.8 | 0.83 | 0.8 | 0.8 | 3.3 | -2.5 |
| b) Croplands | | | | | | | | | | | | | |
| England | 0.95 | 1.1 | 6.3 | 2.1 | 2.1 | -10.5 | -8.4 | 2.11 | 2.1 | 2.1 | 1.1 | 3.2 | -7 |
| Anglia | 0.97 | 4.8 | 2.8 | 0.3 | 1 | 1.4 | -9.5 | 0.6 | 1 | 0.7 | 0.8 | 5 | -4 |
| East midlands | 0.93 | 0 | 1.9 | 0.3 | 1.3 | 1.5 | -9.2 | -0.4 | 4 | 3 | 3.5 | 5 | -4 |
| Wessex | 0.88 | 15 | 5 | 4 | 0.7 | 2.2 | -9 | -0.3 | 5.2 | 3.3 | 3.8 | 4 | -4 |
| South east | 0.92 | 0.16 | 1 | 0.1 | 3 | 0.2 | -1.3 | -0.3 | 4.6 | 7.9 | 8.7 | 6 | -3 |
| Scotland | 0.84 | 2.38 | 2.4 | 2.4 | 0 | 0 | 3.57 | 3.5 | -2.38 | 1.2 | 1.2 | 2.4 | -4.8 |
| N. Ireland | 0.79 | 2.53 | 0 | 1.3 | 2.5 | 0 | -3.8 | 2.5 | -3.8 | 2.5 | 2.5 | 2.5 | -3.8 |
| Wales | 0.81 | -0.86 | -1.23 | 1.9 | 2.5 | -3.7 | -4.9 | 2.5 | 2.5 | -7.4 | 2.5 | 2.8 | -3.7 |

Table 5
Single regression between change in input parameter and average annual N2O emissions.

| Region a) Grasslands | Bulk density (g cm ⁻³) | | Clay content (%) | | Soil pH | | Precipitation (mm) | | Temperature (°C) | | Fertilisation rate (kg N ha^{-1} yr ⁻¹) | |
|-------------------------|------------------------------------|----------------|------------------|----------------|----------------|----------------|--------------------|----------------|------------------|----------------|---|-------------|
| | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) | Mean (+'ve) | Mean (-'ve) |
| England | 0 | 0.03 | 0.04 | 0.02 | 0 | 0.03 | 0.08 | 0.3 | 0.02 | 0.02 | 0.6 | 0.7 |
| Anglia | 0.01 | 0.06 | 0.4 | 0.5 | 0.7 | 0.6 | 0.001 | 0.6 | 0.02 | 0.02 | 0.81 | 0.64 |
| East midlands | 0.1 | 0.06 | 0.19 | 0.2 | 0.58 | 0 | 0.01 | 0.01 | 0 | 0.007 | 0.41 | 0.32 |
| Wessex | 0.55 | 0.4 | 0.61 | 0.63 | 0.3 | 0.2 | 0.01 | 0.01 | 0.02 | 0.02 | 0.56 | 0.5 |
| South east | 0.2 | 0.001 | 0.62 | 0.55 | 0.44 | 0.32 | 0.01 | 0.01 | 0.013 | 0.01 | 0.67 | 0.78 |
| Scotland | 0.13 | 0.02 | 0.007 | 0.02 | 0.1 | 0.17 | 0.02 | 0.4 | 0.02 | 0.02 | 0.23 | 0.36 |
| N. Ireland | 0.06 | 0.59 | 0.05 | 0.05 | 0.1 | 0.31 | 0.04 | 0.57 | 0.34 | 0.36 | 0.66 | 0.74 |
| Wales | 0.37 | 0.53 | 0.51 | 0.47 | 0.56 | 0.52 | 0.02 | 0.08 | 0.27 | 0.18 | 0.77 | 0.87 |
| b) Croplands | | | | | | | | | | | | |
| England | 0.14 | 0.02 | 0.03 | 0.001 | 0.07 | 0.004 | 0.14 | 0.05 | 0.04 | 0.01 | 0.02 | 0.02 |
| Anglia | 0.61 | 0.42 | 0.06 | 0.01 | 0.88 | 0.85 | 0.2 | 0.17 | 0.13 | 0.15 | 0.34 | 0.42 |
| East midlands | 0.02 | 0.02 | 0.01 | 0.001 | 0.72 | 0.7 | 0.24 | 0.21 | 0.27 | 0.29 | 0.16 | 0.3 |
| Wessex | 0.5 | 0.69 | 0.42 | 0.29 | 0.85 | 0.82 | 0.65 | 0.56 | 0.47 | 0.41 | 0.6 | 0.7 |
| South east | 0.02 | 0.01 | 0.3 | 0.34 | 0.25 | 0.25 | 0.51 | 0.45 | 0.66 | 0.7 | 0.37 | 0.4 |
| Scotland | 0.16 | 0.01 | 0.02 | 0.015 | 0.001 | 0.001 | 0.04 | 0.01 | 0.01 | 0.04 | 0.4 | 0.5 |
| N. Ireland | 0.36 | 0.47 | 0.74 | 0.65 | 0.35 | 0.48 | 0.28 | 0.59 | 0.76 | 0.8 | 0.86 | 0.86 |
| Wales | 0.59 | 0.46 | 0.95 | 0.82 | 0.71 | 0.73 | 0.82 | 0.72 | 0.9 | 0.8 | 0.9 | 0.9 |

simulations. For the Monte Carlo simulations, the uncertainty range for each region was based on the characteristics of soils in each of the 1 km² grids within the region, thereby reflecting actual variation, rather than using the arbitrary changes in each input (defined by expert judgement) used in Fitton et al. (2014a,b). While this may lead to unrealistic combinations of different soil inputs being simulated, this approach highlights the importance of both refining input data and the spatial resolution when simulating emissions on a large spatial scale. Soil databases covering large geographical areas tend to use point references and extrapolate to larger scale soil characteristics based on rules or pedotransfer functions (Lilly et al., 2014). Therefore, when N₂O emissions across the UK were initially simulated using the original inputs, it was relatively easy to detect a pattern in the change in emissions, since biogeochemical models like DDC also process and simulate emissions based on fixed rules. This modelling approach highlights the important interactions between soil and climate input parameters on emissions.

The Monte Carlo simulations for grasslands indicated that fertiliser application rates accounted for around 20% of uncertainty. If the importance of N rate on emissions (Bell et al., 2016) is considered, this value may seem low, but can be attributed to the assumption that there

was only a 10% variation in the rates of N applied consistently each year, due to the same management practice being adopted. When a similar ± 10% change in fertiliser application rates was applied to the selected cropland grids, the contribution to uncertainty jumped to approximately 60%. This was because the croplands simulated here were under annual rotation and every year N application rates could range from 80 kg N (\pm 10%) to 0 kg N to 60 (kg N $\,\pm\,$ 10%). Therefore, when averaged over the long term, the actual rate of N applied varies significantly. However, regardless of actual changes in values simulated, annual N₂O emissions tend to be quite sensitive to application rates. While the assumed variation in fertiliser applications rates maybe on the low side, the analysis adopted here demonstrated that for every percentage change in the rate of N applied, either as decrease or an increase, there was a linear response between the two variables. The magnitude of change in N2O emissions was not equal to the change in N application rate. In future, inventory studies should ideally incorporate more refined details of fertiliser management, including type (e.g. urea versus AN), differences in regional application rates, and also differences in the timing of nitrogen application through the growing season.

The modelling approach adopted here was based on the site level analysis described in Fitton et al. (2014a,b). This study describes the

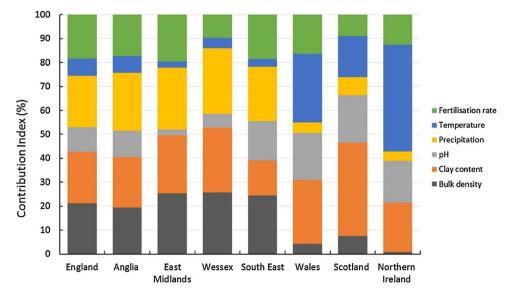
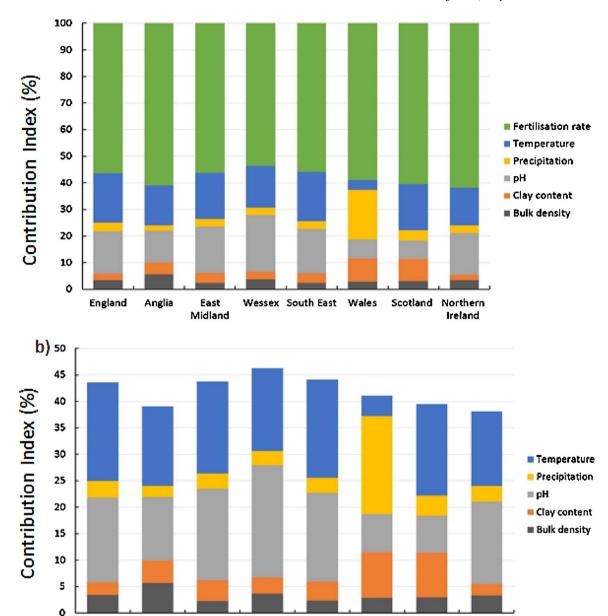


Fig. 4. Contribution index: the contribution (%) of each soil, climate and management input to the range of annual N_2O emissions simulated after the Monte Carlo simulations for UK grasslands in the four regions of the UK: England, Scotland, Wales and Northern Ireland. Values here represent the percentage change in the standard deviation of the range of annual N_2O emissions simulated after the sensitivity analysis of each individual input with respect to the standard deviation of the outputs from the Monte Carlo simulations.



Region

South East

Wessex

Fig. 5. Contribution index: (a) the contribution (%) of each soil, climate and management input to the range of annual N_2O emissions simulated after the Monte Carlo simulations for UK croplands in the four regions of the UK: England, Scotland, Wales and Northern Ireland. (b) the contribution of each input parameter excluding fertiliser. Values here represent the percentage change in the standard deviation of the range of annual N_2O emissions simulated after the sensitivity analysis of each individual input with respect to the standard deviation of the outputs from the Monte Carlo simulations.

successes, advantages and disadvantages of using the DDC model on UK grassland and cropland ecosystems. In terms of advantages the analysis demonstrated that by applying a generic calibration of the DDC model, i.e. not over parameterised to site only conditions, DDC can produce reasonably robust estimated of annual N_2O emissions in response to fertiliser application. Consequently by scaling up the spatial resolution of the annual nitrous oxide emissions, outputs from DDC in this context are relatively accurate (Bell et al., 2015a,b, 2016). There are however some underlying uncertainties in the modelling approaches, at the site level that can feed into spatial estimates. For example, while modelled annual estimates to correlate well with measured values, when daily values are compared model performance deteriorates. This has been

England

Anglia

East

Midland

seen in other studies including Abdalla et al. (2010) and Rafique et al. (2011). Differences in daily values can be attributed to time lags in simulated emissions after N fertiliser application (Li et al., 2005; Del Grosso et al., 2010) and the effect of soil freezing and thawing, especially in winter months (Fitton et al., 2014a; Lit et al., 2010). In addition the processes governing an uptake of N_2O on actively managed grass or croplands are not properly understood (Butterbach-Bahl et al., 2013), therefore as models tend assume/simulate a net release of N_2O this is another source of potential model error (Houska et al., 2017). Other uncertainties arise from the aggregation of input data to spatial girds (Kuhnert et al., 2017).

Northern

Ireland

Scotland

Wales

Internal processes within DDC are also a source of uncertainty of

simulated nitrous oxide emissions. In a study conducted by Brilli et al. (2017), a literature review of the sources of error in different modelling studies was conducted. Based on values reported by different modelling studies, one of the most common causes in uncertainty in modelled N2O emissions from DDC, and also from other models, was uncertainty or incorrectly simulated water filled pore space (WFPS) by the model tended to by the underlying cause of discrepancies between experimental and modelled datasets (Abdalla et al., 2010; Xing et al., 2011; Gabrielle et al., 2006 and Smith et al., 2008). The implementation of management practices by DDC is also a source of error in modelled estimates. Numerous studies have discussed the implication of soil bulk density remaining fixed over time, despite frequent cultivation, especially in croplands, which can lead to an underestimation of the management event on soil C turnover, soil aeration and consequently N2O emissions (Brilli et al., 2017). An inflexibility of how fertiliser is placed on the soil, i.e. spreading, patches or injecting, has also lead to error in modelled outputs as NH₄ and NO₃ which when over or underestimated, have a knock on effect on emissions (Stehfest and Mueller, 2004; Jarecki et al., 2008).

DailyDayCent tends to perform well in model inter-comparisons. Frolking et al. (1998) compared four biogeochemical models on three temperate experimental sites located in the USA, Scotland and Germany. For each set of model simulations, water filled pore space tended to be the most important factor, however, its effect on different N gases varied across the models. Modelled annual emissions from each model at each site tended to be similar to both each other and the experimental datasets, and because of the different causes of uncertainty and errors in different models, increasingly studies adopted a multi model approach or model comparison approach.

Although outside the scope of this study the HWSD and MORECS grid databases provide an excellent framework in which to estimate annual emissions from croplands and grasslands. Advantages of the HWSD database include a) soil and land use is provided to users on a relatively fine spatial scale, and b) soil information to a depth of 1 m. The MORECS grid squares provide users with spatially disaggregated harvest and sowing dates, so they account for climate, for a wide range of crops including spring barley, winter wheat, winter barley, potatoes and others. However, a lack of management activity data for both crops and grasslands is a limitation to the confidence with which DDC, or any other biogeochemical model, can be used. As our results show, especially for croplands, annual emissions can vary as a function of the crop type growing that season. To take advantage of this modelling system, a target for future data collection is spatially disaggregated activity/ management data, which could be used to drive the model. The combination of these improved datasets, with the spatial modelling framework described here, and a multi model ensemble would deliver a powerful Tier 3 system for simulating and reporting N2O emissions from UK agriculture. Other models could be incorporated in the framework to allow a multi-model approach. Furthermore, this type of framework can also be used to provide guidance to policy makers on, for example, targeting of management practices that drive high emissions, in particular regions. In addition it could allow policy makers to test the implications of different mitigation strategies and land use change policies on emissions, both currently and under future possible future climates.

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