Modelling productivity and resource use efficiency for grassland ecosystems in the UK

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\textbf{ABSTRACT}

Estimating spatially resolved grassland productivity is essential for benchmarking the total UK productive potential to assess food, feed and fuel trade-offs in the context of whole systems analyses. Our objectives were to adapt and evaluate a well-known process-based model (PBM) and estimate productivity of improved (permanent, temporary) and semi-natural grassland systems using meta-models (MM) trained by extensive PBM scenario simulations. Observed dry matter (DM) yields in multi-site nitrogen (N) response (0, 150 and 300 kg N ha\textsuperscript{-1}) experiments were well emulated describing the average productivity of rough grazing, permanent and temporary grassland (3.1, 7.4 and 9.8 t DM ha\textsuperscript{-1}, respectively). Cross-validated with independent and long-term data (Park Grass Experiment), the PBM explained more variation when considering all systems combined (81%) than across all improved grasslands (61%) but little for rough grazing (26%). The PBM-trained MM explained 48, 72 and 70% of the simulated yield variation in the grasslands of increasing management intensity, and 43 and 75% of observed variation in the combined improved and all three grassland systems, respectively. Considering the assessment of ecosystem services, like drainage and water productivity, PBM scenario simulations are essential. Compared to improved grassland rough grazing will result in 40% more groundwater recharge due to its lower simulated water use and water productivity (12 versus 25 and 43 kg ha\textsuperscript{-1} mm\textsuperscript{-1} for permanent and temporary grassland, respectively).

\textbf{1. Introduction}

Grasslands constitute a major part of the global ecosystem and contribute significantly to food security (Hopkins and Wilkins, 2006; O’Mara, 2012). In temperate areas of north-western Europe, grasslands can occupy more than 50 percent of the agricultural area (Chang et al., 2015; Peeters, 2004). In the UK, grasslands occupy about two thirds of the agricultural land area (Defra, 2016) and, therefore, are essential for farming systems. Currently, out of 12.4 million hectares (M ha) about 10% were “temporary” grassland (< 5 years old) and of the permanent grassland (> 5 years old) 6.1 M ha are classified as “permanent” pasture and 5.1 M ha as “rough grazing” (Defra, 2016). Especially the latter are very diverse (Allen et al., 2011; Morton et al., 2011), and productivity estimates must be based on management intensity (Hopkins, 2008). In the UK, temporary grassland is highly productive, fertilised and frequently re-sown in rotation with arable crops, permanent grassland is moderately productive and rarely re-sown whilst rough grazing is extensively grazed, low in productivity and never re-sown.

Spatially explicit grassland productivity data are needed to benchmark the UK productive potential and to assess trade-offs between different ecosystem services within a whole systems analysis of bioenergy value chains (Guo et al., 2016; Turley et al., 2010). Grassland productivity is affected by pedo-climatic variables such as soil available water capacity (SAWC), temperature and precipitation (Brereton et al., 1996) and depends on the level of management inputs (Chang et al., 2015). Empirical statistical (and static) weather-yield models have been used to estimate dry matter (DM) yields for arable crops (Chmielewski and Potts, 1995; Lobell et al., 2011) and grassland (Hurtado-Uría et al., 2014; Jenkinson et al., 1994; Trnka et al., 2006). Process-based models (PBMs) simulate dynamics of grass growth and DM yield for different species (Hoglind et al., 2001; Schapendonk et al., 1998) and nitrogen (N) availability (Barrett et al., 2005; Jego et al., 2013). These PBMs were designed for high frequency cutting systems, e.g. silage (Topp and Doyle, 2004) and modified to accommodate low frequency cutting (hay) and grazing systems (Barrett et al., 2005). The adequacy of these PBMs to estimate yield variations across different environments and management systems (e.g. Hurtado-Uría et al., 2013; Persson et al., 2014).
2. Materials and methods

2.1. Experimental systems and data for calibrating and validating the PBM

We considered three systems: temporary grassland, permanent grassland and rough grazing to estimate productivity. Temporary grasslands are the most productive, often consisting of frequently resown perennial ryegrasses (Lolium perenne) and receive a recommended annual N application rate of ca. 300 kg N ha\(^{-1}\) (Defra, 2010). Permanent grasslands consist of a mixture of sown and indigenous grasses and legumes; they are of intermediate productivity and receive moderate inputs (annual N applications of ca. 150 kg N ha\(^{-1}\)). However, these recommended N application rates may not be followed on all temporary and permanent grasslands. The extensively used rough grazing are diverse semi-natural grasslands containing various herbaceous species, receive no synthetic N and are areas of low productivity. In the following these systems are termed temporary (300N), permanent (150N) and rough-grazing (ON).

2.1.1. Dry matter yield data

Annual DM yields for calibration and validation were mainly compiled from two N response experiments at multiple sites in England and Wales (Fig. 1; Table S1). Data came from re-sown temporary grassland after barley on 21 sites between 1970 and 1973 (Morrison et al., 1980) and from permanent and re-sown grassland on four sites between 1983 and 1986 (Murray, 1988). From both sources DM yield data were selected on 300N, 150N and ON plots as proxies for temporary, permanent and rough-grazing grassland, respectively. The respective average DM yields were 9.8, 7.4 and 3.1 t ha\(^{-1}\) (Table 1), the distribution of the measured DM yields on the ON plots was slightly skewed due to some exceptionally high yields caused by residual N from the previous arable crop (Fig. S1). For further validation, long-term DM yields were taken from the ongoing Park Grass Experiment (PGE) at Rothamsted Research, using plots with a ON and 144N treatment from 1960 onward (Fig. S2, plot 3a and 11/1a; ph of 7). These represent respective long-term equilibria for semi-natural and permanent grassland with mixed species and late cutting dates in a wide range of fertiliser and liming treatments (Silverton et al., 2006).

DM yields for further model validation were available for temporary

<table>
<thead>
<tr>
<th>Grassland type</th>
<th>Average</th>
<th>Median</th>
<th>25th</th>
<th>75th</th>
<th>SD</th>
<th>Skewness</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rough-grazing</td>
<td>3.09</td>
<td>3.04</td>
<td>2.02</td>
<td>4.11</td>
<td>1.56</td>
<td>0.51</td>
</tr>
<tr>
<td>Permanent grassland</td>
<td>7.41</td>
<td>7.32</td>
<td>5.79</td>
<td>9.01</td>
<td>2.02</td>
<td>0.04</td>
</tr>
<tr>
<td>Temporary grassland</td>
<td>9.76</td>
<td>9.61</td>
<td>8.34</td>
<td>11.14</td>
<td>2.03</td>
<td>0.01</td>
</tr>
</tbody>
</table>
Table 2
Cutting frequency and dates used to simulate time-series of annual herbage yields by the process-based model for temporary, permanent and rough-grazing grassland, respectively.

<table>
<thead>
<tr>
<th>Grassland</th>
<th>First cut</th>
<th>Second cut</th>
<th>Third cut</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temporary</td>
<td>30 May</td>
<td>20 July</td>
<td>30 Sept</td>
</tr>
<tr>
<td>Permanent</td>
<td>21 June</td>
<td>30 Oct</td>
<td>–</td>
</tr>
<tr>
<td>Rough-grazing</td>
<td>21 June</td>
<td>30 Oct</td>
<td>–</td>
</tr>
</tbody>
</table>

grassland for England (Hopkins et al., 1990; McEwan et al., 1989) and Scotland (Jones et al., 2006). For details see Table S2 and Fig. 1.

2.1.2. Weather data and soil parameters

Locations of UK Met Office weather stations with historic time series of daily records of maximum and minimum temperatures, precipitation, global radiation, relative humidity and wind speed were overlaid with the locations of the experimental sites in ArcGIS (http://www.esri.com/software/arcgis). The closest meteorological station to each experimental site was chosen to represent the respective weather conditions (Table S1). The average distance between the experimental sites and corresponding weather stations was 10.2 km (0.2–29.6 km).

Soil series and SAWC were reported for all sites used by Morrison et al. (1980), whilst soil data for sites used by Murray (1988) and the PGE were taken from the soil map of England and Wales (Table S1). Soil hydraulic parameters needed for the simulation were derived using a pedotransfer function (Woesten et al., 1999).

2.1.3. Management data and assumptions

The experimental treatments of 300N and 150/144N approximate the N requirements of temporary and permanent grassland, respectively (Defra, 2010), and relate to the livestock system and stocking rate as the N requirements of temporary and permanent grassland, respectively (AHDB, 2013).

The experimental site was chosen to represent the respective carbohydrate allocation rates. Elongation rates were determined by generalising the phenology and carbon allocation modules to account for the effects of senescence in extensive and semi-natural grasslands. These modifications affect pheno-morphological development (sink formation) and light interception, photosynthesis and carbohydrate allocation (source formation). Determined by a sink-source balance, the daily growth rate and carbon allocation are limited to the minimum of the sink and source potentials.

2.2. Grass growth model

The sink-source interaction model developed for the growth of small forage grasses (Schapendonk et al., 1998; Hoglund et al., 2001) was implemented into a generic software environment that simulates the water and energy balance (Richter et al., 2006). Originally designed to simulate vegetative growth (Rodriguez et al., 1999) the model was modified by generalising the phenology and carbon allocation modules to account for the effects of senescence in extensive and semi-natural grasslands. These modifications affect pheno-morphological development (sink formation) and light interception, photosynthesis and carbohydrate allocation (source formation). Determined by a sink-source balance, the daily growth rate and carbon allocation are limited to the minimum of the sink and source potentials.

2.2.1. Pheno-morphological development – sink formation

In brief, the model describes leaf emergence, the dynamics of vegetative and generative tillers, and senescence with the translocation of water-soluble carbo-hydrates (reserves) for regrowth. Grass development is determined by the daily accumulation of growing degree days (GDD), starting from 1 January each year. Phenological stages originally defined vegetative growth and tillering using a phyllochron of ca. 100 GDD, and generative tillers being initiated when daily average T exceeded 12 °C (Schapendonk et al., 1998). Stem elongation starts at approximately 900 GDD, the beginning of mid-season peak growth, which culminates in heading at approximately 1600 GDD (Hazard et al., 2006). Cutting sets the phenology back to vegetative growth. Daily GDD is calculated as a function of air temperature against the lower and the upper temperature thresholds (Tb and Tdawnoff °C) for growth. Key growth indices are tiller emergence (GDD), inflorescence (GDD) and maturity (GDDm), which affect translocation of reserves from leaves and stems to seeds and root.

The sink is defined by the potential growth rates of the component plant organs (leaf, stem, and root), which determine the respective allocation demands. The aboveground sink strength is the sum of the potential growth of leaves and stems, which are a function of tiller density, elongation rates and respective morphological parameters, setting the respective carbohydrate allocation rates. Elongation rates are described by a linear function of average daily temperature (Hazard et al., 2006; Hoglund et al., 2001) and affected by water stress described by a logistic function (Sinclair, 1986; Richter et al., 2006). LAI increase is a function of number of simultaneously elongating leaves (ca. three), leaf elongation rate, leaf width, and a leaf shape factor.

Leaf potential growth is calculated based on the LAI increase potential and the specific leaf area (SLA), which is a dynamic variable that ranges between a minimum and maximum to buffer leaf reserves. Stem potential growth is calculated as a function of the stem elongation rate and specific stem weight. The total biomass sink is determined by the dynamics of tiller formation, which is assumed to be a function of leaf emergence rate, the proportion of buds producing new tillers, and the conversion of vegetative to generative tillers.

2.2.2. Light interception and photosynthesis – source formation

The source term consists of water-soluble carbohydrates generated through photosynthetic assimilation of intercepted light and reserve mobilization. Light interception is described as a function of LAI and light extinction, applying Bear’s law (I = I0e(−k*LAI) where I is the canopy-intercepted radiation, I0 the global radiation above the canopy, k the extinction coefficient). The light extinction coefficient, k, is considered a constant, which can range between 0.48 and 0.63 (Hoglund et al., 2005; Schapendonk et al., 1998). In contrast to the
original model (Hoglind et al., 2001; Schapendonk et al., 1998), photosynthesis and respiration are explicitly simulated (Van Laar et al., 1992). Key photosynthetic parameters are the initial quantum efficiency (Φ) and maximum light conversion rate (Amax). Parameter values found in the literature were used to initialize the calibration process (Table 3).

The total source of available carbohydrates to satisfy sink demands is calculated as the net daily integral of the difference between daily leaf photosynthesis and maintenance respiration of the respective organs, plus the mobilisable reserves from leaf, stem, and root biomass. If new assimilates exceed sink demands (Schapendonk et al., 1998), the surplus cascades into reserves and roots. The level of sources (reserves) in the stem and root crown affect tiller formation.

2.2.3. Water productivity

The annual and inter-seasonal dynamics of actual evapotranspiration (ET), drainage and water productivity (WP) were investigated for the different grassland systems. Long-term weather records at Lyneham from 1958 to 2014 were used to run the PBM on six different soil series of contrasting SAWC (Table S3). Annual ET and drainage were accumulated using simulated daily outputs within each hydrological year (1 October to 30 September). The WP was calculated by fitting a simple linear relationship between the respective simulated annual DM yields (kg) and ET (mm).

2.3. Calibrating and up-scaling the PBM

The development of predictive models that can be used at the national scale was made in three steps, as shown in the flowchart (Fig. 2): (A) calibration and validation of the PBM used two subsets of N-dose experiments (Morrison et al., 1980; Murray, 1988) plus long-term datasets from two treatments of the PGE at Rothamsted; (B) building MMs from PBM scenario simulation outputs, Y(PBM), based on multi-site historic weather and soils inputs, using a stepwise forward selection of aggregated pedo-climatic input variables, and finally (C), validation of the MM outputs, Yn(MM), using two cases of independent observations for pedo-climatic variables and DM yields, Y(O).

2.3.1. Calibrating and validating PBM

Step A: Among the sites of the N-dose experiments, the first subset of 10 sites was selected (Table S1; “.cal”) to calibrate the most important parameters of the PBM influencing grass growth (Table S4). The initial values of these were set to default photosynthetic and morphological parameters taken from the literature (Table 3) and calibrated to reflect the relative productivity in response to N supply. Parameters were calibrated for the respective grassland types by iteration minimising the RMSE and bias of simulated versus observed DM yields. The remaining 15 sites of the N-dose experiments (Table S1) were used to validate the calibrated PBM. In addition, the 0N and 144N treatments of the PGE were used to validate the long-term yields of rough grazing and
permanent grassland, respectively.

2.3.2. Up-scaling the PBM

2.3.2.1. Simulation scenarios to generate multi-site DM yields. Step B1: The PBM was up-scaled using long time series of weather records from six representative weather stations across England and Wales to vary annual grassland yields across a wide range (Hurtado-Uria et al., 2014; Jenkinson et al., 1994). The scenarios were simulated using a generic set of soils across a wide range of SAWC (50–196 mm) and also soils reported in the original datasets (Table S3). The soil parameters for the PBM were derived by applying the procedure described by Lovett et al. (2009), based on primary soil physical properties (texture, bulk density and soil organic matter content) to calculate soil water retention and SAWC of each layer within the rooting depth.

The distribution of the aggregated soil hydrological and climatic variables derived from the historic weather records varied considerably within and between sites (Table S5). SAWC varied by a factor of two to five. The variability of precipitation increased during the summer, June/July and August/September ranging between ca. 20 mm to more than 200 – 300 mm. Such span in precipitation was matched by average monthly summer temperatures varying between 13 and 19 °C. Monthly irradiation varied more during spring (665–1395 MJ) than summer (538–914 MJ).

2.3.2.2. Aggregating input variables. Step B2: As temporary grasslands had three cuts, bioclimatic variables were aggregated across three growth phases: cumulative precipitation (PAMJ) and global radiation (RAMJ), and mean air temperature (TAMJ) for March to May; cumulative precipitation (PJAS) and global radiation (RJAS), and mean air temperature (TJAS) in June and July; and finally cumulative precipitation (PAS) and global radiation (RAS), and mean air temperature (TAS) in August and September. As permanent and rough-grazing grasslands had two cuts, bioclimatic variables were aggregated over two growing periods, April to June and July to September: input variables consisted of cumulative precipitation (PAMJ, PJAS), cumulative global radiation (RAMJ, RJAS), but mean air temperature in March to May (TAMJ), and July to September (TJAS).

2.3.2.3. MM derivation. Step B3: Coefficients of the MMs were derived by fitting regressions using stepwise variable selection of the aggregated biophysical variables in Genstat (Payne et al., 2011) against the dependent variable DM yield, generated in the scenario simulations, Y(PBM). The selection of the MMs’ candidate variables was optimised to explain the maximum variation of scenario yields. Variables included site-specific SAWC and aggregated bioclimatic variables, monthly mean temperature (ØT_{m}), monthly totals of precipitation (∑P_{m}) and global radiation (∑R_{m}) during the respective phases of the growing season. These phases for aggregating bioclimatic variables depended on the sward management (time and frequency of cutting, Table 2). The fitted multiple regression model consisted of a linear combination of grass growth-determining biophysical variables as follows:

\[ Y_{M} = a + \sum_{1}^{n} b_{i} V_{i} + \epsilon \]  

in which \( Y_{M} \) is the MM fitted/estimated DM yield, \( V_{i} \) represents the number of predetermined soil physical and aggregated bioclimatic variables from 1 to \( n \), \( \epsilon \) is the error term, and \( a \) and \( b_{i} \) are regression coefficients to be estimated. Quadratic terms of SAWC and aggregated precipitation were included after determining the most appropriate linear combination of necessary soil and aggregated bioclimatic variables using a t-test for the coefficient estimate and an F-test for the reduction in residual mean squares during a forward stepwise regression.

2.3.3. MM evaluation

Step C: MM outputs were evaluated against PBM scenario outputs and against their subsets of PBM simulated yields at the experimental sites. The main MM evaluation, however, compared MM estimates against observed DM yields for two cases (A and B in Fig. 3):

- Case A: MM-estimated DM yields evaluated against observed DM yields at the 25 experimental sites of multi-year experiments (Morrison et al., 1980; Murray, 1988) and the observations in the PGE (Ex01-25; Ex26; Table S1; \( n = 446 \))
- Case B: MM-estimated DM yields evaluated against observed DM yields in multi-year experiments on temporary grassland at 15 independent sites (Table S2; \( n = 178 \)). Among these sites, 14 sites provided annual DM yields from 4-week cutting intervals (Hopkins et al., 1990; McEwen et al., 1989) while the remaining site provided annual DM yields from three cuts per year which corresponds to 8-week cutting intervals.

2.4. Model performance indicators

Of the indicators proposed for model evaluation (Smith et al., 1997) the following statistical indicators were calculated to assess the goodness-of-fit between modelled and observed DM yields:
Table 4
Performance indicators of model goodness of fit in calibrating and validating the PBM for temporary (TG), permanent (PG) and rough-grazing (RG) grasslands in multi-site experiments: residual mean square error (RMSE), relative root mean square error (RMSE%), mean bias error (MBE), mean relative bias (MBE%) and variance accounted (% adjusted $R^2$). The indicators of model goodness of fit were calculated for separate and combined simulated DM yields compared to observed DM yields, $Y(O)$. $\overline{Y}$ is the mean annual DM yield calculated from observations at the selected sites of multi-year experiments; $n =$ number of observations.

<table>
<thead>
<tr>
<th>Data case</th>
<th>Grassland</th>
<th>$\overline{Y}$ (t ha$^{-1}$)</th>
<th>RMSE (t ha$^{-1}$)</th>
<th>MBE (t ha$^{-1}$)</th>
<th>RMSE% (%)</th>
<th>MBE% (%)</th>
<th>Adjusted $R^2$</th>
<th>$n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calibration 10 sites</td>
<td>TG</td>
<td>9.1</td>
<td>1.53</td>
<td>-0.54</td>
<td>16.76</td>
<td>13.58</td>
<td>63.9</td>
<td>43</td>
</tr>
<tr>
<td></td>
<td>PG</td>
<td>6.2</td>
<td>1.62</td>
<td>-0.33</td>
<td>25.93</td>
<td>23.15</td>
<td>50.1</td>
<td>43</td>
</tr>
<tr>
<td></td>
<td>RG</td>
<td>2.7</td>
<td>1.68</td>
<td>0.48</td>
<td>62.62</td>
<td>73.01</td>
<td>28.9</td>
<td>43</td>
</tr>
<tr>
<td></td>
<td>TG + PG</td>
<td>7.7</td>
<td>1.57</td>
<td>-0.44</td>
<td>20.49</td>
<td>18.37</td>
<td>70.1</td>
<td>86</td>
</tr>
<tr>
<td></td>
<td>TG + PG + RG</td>
<td>6.0</td>
<td>1.61</td>
<td>-0.13</td>
<td>26.79</td>
<td>36.58</td>
<td>80.1</td>
<td>129</td>
</tr>
<tr>
<td>Validation 15 sites + PGE</td>
<td>TG</td>
<td>10.1</td>
<td>1.66</td>
<td>-0.44</td>
<td>16.34</td>
<td>13.42</td>
<td>28.4</td>
<td>69</td>
</tr>
<tr>
<td></td>
<td>PG</td>
<td>7.8</td>
<td>1.55</td>
<td>0.05</td>
<td>19.77</td>
<td>16.77</td>
<td>39.3</td>
<td>124</td>
</tr>
<tr>
<td></td>
<td>RG</td>
<td>3.2</td>
<td>1.31</td>
<td>0.47</td>
<td>40.50</td>
<td>41.74</td>
<td>21.6</td>
<td>124</td>
</tr>
<tr>
<td></td>
<td>TG + PG</td>
<td>8.6</td>
<td>1.59</td>
<td>-0.12</td>
<td>18.36</td>
<td>15.57</td>
<td>52.8</td>
<td>193</td>
</tr>
<tr>
<td></td>
<td>TG + PG + RG</td>
<td>6.5</td>
<td>1.49</td>
<td>0.11</td>
<td>22.74</td>
<td>25.81</td>
<td>81.5</td>
<td>317</td>
</tr>
<tr>
<td>Calibration + Validation</td>
<td>TG</td>
<td>9.8</td>
<td>1.57</td>
<td>-0.45</td>
<td>16.10</td>
<td>13.15</td>
<td>49.9</td>
<td>112</td>
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<td></td>
<td>PG</td>
<td>7.4</td>
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<td>18.34</td>
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<td>167</td>
</tr>
<tr>
<td></td>
<td>RG</td>
<td>3.1</td>
<td>1.42</td>
<td>0.47</td>
<td>45.87</td>
<td>49.79</td>
<td>25.9</td>
<td>167</td>
</tr>
<tr>
<td></td>
<td>TG + PG</td>
<td>8.4</td>
<td>1.56</td>
<td>-0.21</td>
<td>18.71</td>
<td>16.25</td>
<td>60.9</td>
<td>279</td>
</tr>
<tr>
<td></td>
<td>TG + PG + RG</td>
<td>6.4</td>
<td>1.51</td>
<td>0.05</td>
<td>23.68</td>
<td>28.81</td>
<td>81.3</td>
<td>446</td>
</tr>
</tbody>
</table>

Mean bias error (Eq. (2)), relative mean absolute bias error (% Eq. (3)), root mean square error (Eq. (4)), relative root mean square error (%, Eq. (5)) and the adjusted $R^2$ statistic (Eq. (6)) were calculated for separate and combined simulated DM yields compared to observed DM yields, $Y(O)$. $\overline{Y}$ is the mean annual DM yield calculated from observations at the selected sites of multi-year experiments; $n =$ number of observations.

$$ MB E = \frac{1}{n} \sum_{i=1}^{n} Y_{obs} - Y_{est} $$ (2)

$$ MB E % = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{Y_{obs} - Y_{est}}{Y_{obs}} \right) * 100 $$ (3)

$$ RM SE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (Y_{obs} - Y_{est})^2 } $$ (4)

$$ R M S E % = \frac{RM SE}{\overline{Y}} * 100 $$ (5)

Adjusted $R^2$ was used as a criterion for crop growth model performance (Jamieson et al., 1991) establishing thresholds for model performance to be "excellent", "good", "fair" and "poor" with RMSE % ≤ 10%, 10% < RMSE% ≤ 20%, 20% < RMSE% ≤ 30%, and RMSE% > 30%, respectively.

The percentage variance accounted for (i.e. adjusted $R^2$; Eq. (6)) uses the residual mean square (MS) and total mean square (Total MS) when observed DM yields (dependent variable) were linearly related to estimated DM yields (independent variable):

$$ adjusted R^2 = 100 \left( 1 - \frac{\text{Residual MS}}{\text{Total MS}} \right) $$ (6)

3. Results

3.1. Parameterizing the PBM for different grassland types

3.1.1. Calibration

Fig. 3a shows the relationship between the measured and simulated DM yields for the proxy of temporary, permanent and rough grazing grasslands in the calibration (Set 1, 10 sites) of N-dose experiments (Table S1). The variance accounted for was 63.9, 50.1 and 28.9%, respectively (Table 4). While the bias was small (MBE of 0.3–0.5 t ha$^{-1}$), and the error acceptable (RMSE around 1.5 and 1.7 t ha$^{-1}$), for all grassland types, the mean relative bias was high (73.3%) for rough grazing compared to temporary and permanent grassland (13.6 and 23.2%, respectively). When yields were combined for both temporary and permanent or all three grassland types, the variance accounted for increased to 70.1 and 80.1%, respectively (Table 4), due to the productivity difference. Excluding rough-grazing, the RMSE% of 16.76% for temporary and 25.93% for permanent grassland were within the acceptance criteria of good and fair model performance, respectively.

3.1.2. Validating the parameterised PBM

For the validation subset (15 of 25 of N-dose experiment sites plus PGE) the simulations with the calibrated PBM compared well overall to the observed DM yields across all three types of grassland (Fig. 3b). The PBM explained 28.4, 39.3 and 21.6% of the variance in temporary, permanent and rough grazing grasslands, respectively (Table 4). The MBE was < 0.5 t ha$^{-1}$ and the RMSE was about 1.5 t ha$^{-1}$ for all grass types. The MBE%
3.2. Scenario DM yields for different grassland systems

Based on the chosen cutting frequencies and dates (Table 2) and the calibrated parameters for the different grassland systems (Table 3), panels of long-term time-series of DM yields were generated using the PBM. These simulated DM yields for the different grassland systems were distributed over a large overlapping range, especially for the productive (temporary and permanent) grasslands, but each system has a distinctly different peak probability (Fig. 4).

3.2.1. Regulating water use and groundwater recharge

In these scenario simulations, the annual simulated actual ET depends on SAWC and grassland type (Fig. 5a). It was similar in temporary and permanent grassland but lower under rough grazing (see also Table S6). It is likely that in reality an even greater difference between the grassland systems can be expected as temporary grassland is located on soils with high SAWC, whilst rough grazing is found on shallow soils with low SAWC. Like annual ET, annual drainage was grassland type specific and strongly dependent on the SAWC (Fig. 5b). The annual drainage was similar in temporary and permanent grassland, and smaller than under rough grazing (Table S6), which is an important result to discuss in terms of groundwater recharge.

3.2.2. Resource use efficiency – water productivity (WP)

WP was calculated by fitting a simple linear relation between the annual DM yield and the respective annual ET. The results (Table 5 and Fig. 6) show clearly, that WP was almost four times higher in the highly productive grasslands than in rough-grazing. On average, WP was estimated to be 42.6, 25.0 and 11.8 kg ha\(^{-1}\) mm\(^{-1}\) for temporary and permanent grasslands and rough-grazing, respectively.

Table 5

<table>
<thead>
<tr>
<th>Grassland</th>
<th>a (kg ha(^{-1}) mm(^{-1}))</th>
<th>b (kg ha(^{-1}) mm(^{-1}))</th>
<th>Adjusted R(^2) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temporary</td>
<td>-2124.1 (391.0)</td>
<td>42.6 (1.33)</td>
<td>75.3</td>
</tr>
<tr>
<td>Permanent</td>
<td>-198.1 (98.3)</td>
<td>25.0 (0.96)</td>
<td>66.6</td>
</tr>
<tr>
<td>Rough grazing</td>
<td>-48.3 (98.3)</td>
<td>11.8 (0.44)</td>
<td>67.9</td>
</tr>
</tbody>
</table>

3.3. Deriving MMs for different grassland systems

3.3.1. Variable selection

Exploring pedo-climatic variables during the active growing season, SAWC within rooting depth was found to be a significant input variable for all grassland management types. The forward stepwise variable selection in the regression procedure identified SAWC and the following aggregated bioclimatic variables (see Eqs. (7)-(9)) necessary to be included. The estimated regression coefficients are given in the equations below and the respective statistics are shown in the supplemental information (Table S7). The derived MMs for annual DM yields were the following:

Temporary grassland, YM(TG):

\[
YM(TG) = -2.18 + 0.1267*SAWC - 0.00315*SAWC^2 
+ 0.04013*PAMAM - 0.0000949*PAMAM^2 + 0.05079*PMJ 
- 0.0001204*RAMJ + 0.02704*PAS 
- 0.0000717*PAS^2 - 0.0002917*PASM + 0.7105*TMAM 
- 0.00002261*SAWC^2 + 0.004381*PAMJ - 0.0000945*PAMJ^2 + 0.03457*PAS 
- 0.0004871*PASM - 0.0002489*RASM + 0.002826*RJAS 
+ 0.1877*TMAM - 0.0808*TJAS 
(7)
\]

Permanent grassland, YM(PG):

\[
YM(PG) = -2.915 + 0.09914*SAWC - 0.0002261*SAWC^2 
+ 0.04381*PAMJ - 0.0000945*PAMJ^2 + 0.03457*PAS 
- 0.00004871*PASM - 0.0002489*RASM + 0.002826*RJAS 
+ 0.1877*TMAM - 0.0808*TJAS 
(8)
\]

Rough-grazing grassland, YM(RG):

\[
YM(RG) = -0.862 + 0.03865*SAWC - 0.0001028*SAWC^2 
+ 0.0146*PAMJ - 0.00003894*PAMJ^2 + 0.01294*PAS 
- 0.00002482*PASM - 0.0000935*RJAS 
+ 0.035*TMAM - 0.1046*TJAS 
(9)
\]

The variance accounted for was 69.6, 72.2 and 47.6% for temporary
ary, permanent and rough grazing grassland, respectively.

3.3.2. Validating meta-models

Under Case A, the MM-predicted DM yields were validated against DM yields measured in all 25 sites of N-dose experiments and data from the PGE (Fig. 7a; Case A in Table 6). Except for rough-grazing, the RRMSE% identified a “fair” model performance for temporary (21.1%) and permanent (24.0%) grassland. However, the MM predictions for rough grazing fitted observed DM yields in the PGE alone better than when pooled with the 25 sites of the N-dose experiment: the RRMSE% improved from 24.0 to 20.5%.

When the MM was validated against observed DM yields in temporary grassland only (receiving 300 kg N ha\(^{-1}\)) at 15 independent sites (Fig. 7b) the goodness of fit showed an increased error (RMSE > 2 tha\(^{-1}\)) but negligible bias (Table 6, Case B). Overall, the model performance was fair (RRMSE% = 23.8%). Some of the error could be clearly attributed to high DM yields in the first harvest year after re-seeding (filled symbols).

4. Discussion

4.1. Predictive power of the PBM

To the best of our knowledge, this is the first time that a PBM has been evaluated for such a comprehensive data set that covered all relevant grassland systems. Their productivities are well described by a widely used sink-source interaction model adapted here to respond to environmental factors (Hurtado-Uria et al., 2014) and level of N fertilisation (Hopkins et al., 1990; Hopkins et al., 1995; McEwen et al., 1989). The different input/output regimes of the selected grassland types were modelled calibrating parameters dependent on

Fig. 6. The relationship between simulated annual DM yield and evapotranspiration within the growing season using the calibrated PBM on temporary (a), permanent (b), and rough-grazing grassland (c) simulated using historic weather records (1958–2014) at Lyneham on six soil types of different SAWC (mm).

Fig. 7. Evaluation of DM yields estimated by meta-model, Y(MM), against observed DM yields, Y(O), Table 6; (a) Case A: observed for all grassland types at 25 sites of the multi-year experiments (open symbols) and for rough-grazing (▲) and permanent grassland (■) observed on the PGE; (b) Case B: observed at 15 sites of multi-year experiments for temporary grassland (◊, McEwen et al., 1989), (▽, Jones et al., 2006) and (○, Hopkins et al., 1990) – solid circles (●) represent first yields after re-seeding.
The performance indicators of model goodness of fit for MM-fitted DM yields, $Y$(MM), for compared to observed DM yields (Case A) for temporary (TG), permanent (PG) and rough-grazing (RG) at the 25 sites of the multi-year experiments plus PGE used for calibration and validation of the PBM (Table S1; Fig. 7a), and (Case B) Temporary Grassland at 15 independent experiments (Table S2, Fig. 7b). $\bar{Y}$ is the mean annual DM yield calculated from observations at the selected sites of multi-year experiments.

<table>
<thead>
<tr>
<th>Case</th>
<th>Grassland</th>
<th>$\bar{Y}$ (t ha$^{-1}$)</th>
<th>RMSE (t ha$^{-1}$)</th>
<th>MBE (t ha$^{-1}$)</th>
<th>RRMSE%</th>
<th>MBE%</th>
<th>Adjusted $R^2$</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>A (25 sites + PGE)</td>
<td>TG</td>
<td>9.76</td>
<td>2.66</td>
<td>−0.359</td>
<td>21.15</td>
<td>18.57</td>
<td>25.7</td>
<td>112</td>
</tr>
<tr>
<td></td>
<td>PG</td>
<td>7.41</td>
<td>1.78</td>
<td>-0.056</td>
<td>24.03</td>
<td>20.63</td>
<td>29.6</td>
<td>167</td>
</tr>
<tr>
<td></td>
<td>RG</td>
<td>3.09</td>
<td>1.50</td>
<td>0.593</td>
<td>48.57</td>
<td>53.42</td>
<td>22.0</td>
<td>167</td>
</tr>
<tr>
<td></td>
<td>TG + PG</td>
<td>8.36</td>
<td>1.90</td>
<td>-0.178</td>
<td>22.72</td>
<td>19.80</td>
<td>43.3</td>
<td>279</td>
</tr>
<tr>
<td></td>
<td>TG + PG + RG</td>
<td>6.38</td>
<td>1.76</td>
<td>0.111</td>
<td>27.60</td>
<td>32.39</td>
<td>74.7</td>
<td>446</td>
</tr>
<tr>
<td>B (15 sites)</td>
<td>TG</td>
<td>10.24</td>
<td>2.44</td>
<td>-0.01</td>
<td>23.84</td>
<td>19.08</td>
<td>13.28</td>
<td>178</td>
</tr>
</tbody>
</table>

N input, e.g. tiller numbers and photosynthesis (Table 3; Johnson et al., 1983) and N off-take (Morrison et al., 1980). The choice of experimental sites represented grasslands of all climate regions in Great Britain (Fig. 1) and soils of diverse fertilities as indicated by the wide range of respective DM yields on the ON plots at different sites (Morrison et al., 1980). Using long-term weather data for the scenario simulations its validity and derived MM expanded well into Scotland (Jones et al., 2006).

Other key management variables distinguishing grassland systems were cutting regime (Herrmann et al., 2005), as temporary grassland is likely to be harvested twice early for silage, whilst permanent grasslands may have one later silage or hay cut, both followed by grazing (Table 2). Grazing only can be mimicked by frequent cutting (Barrett et al., 2005) although growth pattern is different (Hurtado-Uría et al., 2014; Orr et al., 2001). This paper doesn’t aim to quantify the effects of grazing but to distinguish grassland types according to management intensity. The model was, therefore, better at estimating productivities for improved (temporary and permanent) than semi-natural grassland, whilst fitting their mean productivities well (Fig. 3; Table 4). Poorer model performance for rough-grazing was partly attributed to high yields (> 6 t ha$^{-1}$) in the first harvest year due to N carried over from previous barley crops and partly to many low yields (< 2 t ha$^{-1}$) in soils of poor fertility (Fig. 3, Fig. S1). Strictly speaking, this is a “temporary grassland” artefact, also observed in re-sown grassland (Hopkins et al., 1990; Fig. 7b). When excluded from evaluations, the “rough grazing” analogue (Section 3.1.2) compared much better, especially to observed yields in the PGE (MBE% and RRMSE%) were reduced from 41.7 to 23.2% and 40.5 to 26.7%, respectively). Overall, however, the used PBM greatly simplified the diversity encountered in mixed grassland (Jouven et al., 2006; Topp and Doyle, 2004).

4.2. Meta-models versus process-based model

Whilst PBMs describe the interactions of physiological and morphological mechanisms controlled by environmental and management variables, MM linearize these mechanisms and ignore interactions. MM estimates accounted for less variation of observed DM yields than the PBM (Tables 4 and 6). Overall, the MM validations were slightly noisier and an overall decrease in certainty of < 10% was observed. This can be partly attributed to the conversion of daily weather into aggregated bi- or tri-monthly input variables during critical growth phases. Nevertheless, the coefficients estimated for the MM variables were meaningful (Table S7) and produced predictions in good agreement with observed yields (Table 6, Fig. 7). Once PBMs are validated for a large range of pedo-climatic (weather x soil) and eco-physiological conditions, the MMs derived from these PBM scenario outputs can reliably approximate productivities. They are biophysically meaningful when SAWC in the root zone and bioclimatic variables are combined (Lobell and Burke, 2010; Phelan et al., 2016).

Due to the uncertainty of spatially resolved inputs over large regions, MMs are considered sufficiently precise and increase the simplicity of GIS-based computations. Such spatially resolved productivity data approximate the reality and can be used for exploratory mapping (Chang et al., 2015; Liu et al., 2011; Lovett et al., 2014). Caution must be exercised for the likely use of MMs outside the range of biophysical variables, which was compensated for by using a wide range of scenario inputs (Step B1, Fig. 2), to ensure the validity for climate change scenarios.

Nevertheless, MMs have two limitations: first, they cannot be transferred to different management systems, and second, they are limited to a single output and give no information on other ecosystem services (e.g. water balance). They are static and for limited range of time and place, “there and then”, because their estimated coefficients are empirical. Contrary to this, PBMs are dynamic and estimates can be both “there and then” and “here and now” (real time) because parameters are based on eco-physiological understanding. Nevertheless, it is concluded that both, the PBM and MM reflect productivity of grasslands with variable management (Figs. 3 and 7).

4.3. Up-scaling opportunities and limitations

PBMs usually need high quality inputs (especially weather), which rarely exist for large regions (Van Bussel et al., 2011). The question arises whether the use of a complex dynamic model is justified over the fast MM derived from PBM simulations or “simulated observations” (Lobell and Burke, 2010). Validation against real observations (Figs. 7) improves the confidence in our MM approach, which can be considered to be a robust yield estimate at large scale (Soltani et al., 2016), similar to statistical weather-yield models established from observations only (Richter et al., 2008). Our MMs for baseline grassland productivity were derived from multi-site panel simulations (Lobell and Burke, 2010) without the need of de-trending. For future productivities all other yield effects, e.g. technology advance and climate change can be applied externally. Although PBMs come with less uncertainty, its gain over yield estimates from MMs was not significant (p > 0.05 when paired-t test was conducted).

However, PBMs incorporate more functionalities such as flow of water and nutrients in the soil-plant-atmosphere continuum. PBMs provide dynamic understanding of productivity gains and environmental trade-offs whereas MMs estimate production only. The usage of PBMs is justified for multi-purpose outputs, as exemplified for WP (see 3.2.2). For other outputs one needed to revisit PBMs, as shown for hydrological ecosystem services here.

4.4. Regulating water regime

Drainage, ET and WP are service indicators of regulating water regimes in agroecosystems (Maxwell and Condon, 2016; Moot et al., 2008; Nielsen et al., 2006). Annual ET was smaller for rough-grazing compared with temporary and permanent grasslands, due to a smaller LAI and a slower build-up of the canopy. Under rough-grazing, the plant community will differ from temporary and permanent grassland.
Rough-grazing land is usually poor in nutrients, which results in limited tillering and leaf extension (Clark et al., 2014; Martinefsky et al., 2010) which is reflected in its PBM parameters (Table 3). Here, a double effect becomes apparent as actual ET is increasing up to an SAWC of 110 mm, where it is levelling off (Fig. 5a) separating marginal from fertile soils; conversely, annual drainage decreased up to an SAWC of about 110 mm (Fig. 5b). The level of ET is lower under rough grazing than improved grasslands, creating on average more groundwater recharge, which is an important ecosystem service to be considered in the context of choosing perennial vegetation (Hamilton et al., 2015).

Biomass-based WP reflects the management conditions (Steduto et al., 2007). WP of temporary grassland calculated here is slightly higher than that for forage from Triticale (32.2 kg ha\(^{-1}\) mm\(^{-1}\); Nielsen et al., 2006) or cocksfoot (Dactylis glomerata) with 38 and 17 kg ha\(^{-1}\) mm\(^{-1}\) for the 300N and ON treatments, respectively (Moot et al., 2008), which were in close agreement with estimates for similar treatments here (Fig. 6; Table 5).

4.5. Relevance

For optimising land use it is important to spatially differentiate productivity for different grassland systems, both locally and nationally (Chang et al., 2015; Guo et al., 2016; Turley et al., 2010). Production potentials need to be benchmarked for whole system trade-offs using land for conservation and other ecosystem services (Hopkins and Holz, 2006; Leimer et al., 2015; McEwen et al., 1989; Smit et al., 2008). Here, we referred to modelled grassland productivity as annual potential DM yield for feed, biogas feedstock or for extensive grazing. Productivity is strongly dependent on SAWC and weather, and both modelling yields for feed, biogas feedstock or for extensive grazing. Productivity is strongly dependent on SAWC and weather, and both modelling approaches conserve these relationships for different grassland systems. High forage productivity requires adequate N, and the 300N treatment used here for temporary grassland was within the economic optimum of N across the UK (Morrison et al., 1980). Higher productivity is possible with new grass species and higher input but often uneconomical (Hopkins et al., 1990) and environmentally detrimental (del Prado et al., 2006). Other factors than N supply (other nutrients, irrigation, diseases, pests, weeds and cutting/grazing frequency (Hopkins et al., 1995; McEwen et al., 1989) have been ignored here. However, the effect of phosphorus availability is accounted for in tiller densities across different systems (Table 3).

Overall, our results closely reflect the reality of grassland productivity of rough-grazing (2–3 t ha\(^{-1}\); Hopkins, 2008), permanent grassland with moderate N inputs from fertiliser or legumes (7–9 t ha\(^{-1}\)) and temporary grassland (10–12 t ha\(^{-1}\); AHD, 2013). Average yield measured in the PGE were similar with 3.2 (± 1.1) and 8.5 (± 1.7) t ha\(^{-1}\) for rough (ON) and improved (144N) permanent grassland and stable over 55 years (Fig. S2). Respectively productivities of permanent and rough grazing grasslands usually reach 80 and 10% of temporary grassland (Chang et al., 2015). In the UK, however, the productivity of rough-grazing grasslands reaches about 20%, as the average biomass yields of the scenario simulations show for the three systems (10.50 (± 2.84), 7.29 (± 2.25) and 2.25 (± 0.70) tha\(^{-1}\)). The MMs are being up-scaled to estimate national feedstock based on spatially differentiated inputs for soil, land cover (Morton et al., 2011) and land use constraints (Lovett et al., 2014). Future predictions will account for climate change projections (UKCP09) and technological progress including advances in breeding and crop management (Smit et al., 2008; Chang et al., 2015).

5. Conclusions

For grassland, the largest land use system in the UK, a PBM was parameterised and evaluated using a large set of N-dose experiments at multiple sites to estimate productivities of all grassland systems. Up-scaled to statistical MMs derived from PBM scenario of multi-site panel simulations (soil types x long-term weather) the predictive ability of these MMs for temporary and permanent grassland systems was similar to the PBM. The MMs are therefore an effective tool to scale up the PBM to provide spatially explicit productivity over large regions for the baseline and future scenarios. Taking into account the respective areas of each grassland type, the total annual biomass of UK grassland could be about 70 million tonnes of DM with a considerable option for biogas production. Outputs regarding multiple ecosystem services, MBBMs seem indispensable to assess resource use efficiency and ground water recharge (drainage), and possibly impacts of increased N fertiliser inputs.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.eja.2017.05.002.

References
