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Modelling biological N fixation and grass-legume dynamics with process-based biogeochemical models of varying complexity



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ABSTRACT

Grasslands comprised of grass-legume mixtures could become a substitute for nitrogen fertiliser through biological nitrogen fixation (BNF) which in turn can reduce nitrous oxide emissions directly from soils without negative impacts on productivity. Models can test how legumes can be used to meet environmental and production goals, but many models used to simulate greenhouse gas (GHG) emissions from grasslands have either a poor representation of grass-legume mixtures and BNF, or poor validation of these features. Our objective is to examine how such systems are currently represented in two process-based biogeochemical models, APSIM and DayCent, when compared against an experimental dataset with different grass-legume mixtures at three nitrogen (N) fertiliser rates. Here, we propose a novel approach for coupling DayCent, a single species model to APSIM, a multi-species model, to increase the capability of DayCent when representing a range of grass-legume fractions. While dependent on specific assumptions, both models can capture the key aspects of the grass-legume growth, including biomass production and BNF and to correctly simulate the interactions between changing legume and grass fractions, particularly mixtures with a high clover fraction. Our work suggests that single species models should not be used for grass-legume mixtures beyond about 30% legume content, unless using a similar approach to that adopted here.

1. Introduction

Biological nitrogen fixation (BNF) is the source of large annual additions of nitrogen (N) to the terrestrial biosphere. Despite the importance of manufactured fertilisers in crop production, inputs of N from BNF to the terrestrial environment have been estimated to be more than double that from fertiliser inputs (Fowler et al., 2015; Galloway et al., 2004). It is also predicted that by the end of the current century, BNF in agricultural systems will increase from 33 to

65 Tg N y⁻¹ as a consequence of demand for increased production and climate change (Fowler et al., 2015). This is partly credited to an attempt to increase the utilisation of BNF in agricultural systems due to a perceived benefit in environmental outcomes.

For example, there is evidence that greenhouse gas (GHG) emissions from N derived from BNF are lower than those associated with manufactured fertilisers, particularly as a consequence of lower nitrous oxide (N₂O) emissions (Jensen et al., 2012; Rochette and Janzen, 2005). As N₂O concentrations have increased (Bates et al., 2008), and indirect

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emissions of N₂O caused by mineral fertiliser in agriculture now account for 35–54% of total N₂O emissions (Davidson, 2009; EPA, 2006). Mitigation scenarios for grasslands that propose as a way of reducing N₂O emissions (Smith et al., 2008; de Klein and Eckard, 2008) are important. This includes the use of legumes, which purportedly provide a better synchronicity of N supply and plant N uptake and thus reduce the requirement for N fertiliser. In a meta-analysis, Jensen et al. (2012) demonstrated that N₂O emissions across several sites were reduced as the fraction of legumes increased and the N fertiliser use declined. However, it was not clear from that meta-analysis whether the reduced N₂O emissions were accompanied with a loss of productivity. Theoretically, N₂O emissions could be reduced, as fertiliser application increases the amount of available N within the soil leading to “hot spots” which characterise N₂O emissions (Butterbach-Bahl et al., 2013). Therefore, the most desirable mitigation strategy is one that reduces N₂O emissions without compromising agricultural production. The presence of legumes offers the potential to improve the balance between N supply and plant N uptake. Recently, Lüscher et al. (2014) argued that legume-based grassland systems could have higher productivity at lower cost and N₂O emissions than grass-only systems using N fertilisers and that this can be best achieved with a sward containing 30–50% legumes (Lüscher et al., 2014).

Models provide a potentially valuable tool to test this kind of theory and offer a chance to explore the best ways in which legumes can be used to meet environmental and production goals. Unfortunately, many models that are widely used to simulate GHG emissions from grasslands have either a poor representation of grass-legume mixtures and BNF, or poor validation of these features (Snow et al., 2014; Kipling et al., 2016). These include widely used models such as DayCent (Parton et al., 1998) and APSIM (Holzworth et al., 2014), which are commonly used to estimate GHG emissions and mitigation options (Ehrhardt et al., 2018). Given the lack of validation and poor implementation of legume-grass systems in models, our objective was to examine how such systems are currently represented in two process-based biogeochemical models, APSIM and DayCent, and improve their capability where required. Therefore, the principal aim of this study was to test the capacity of structurally different biogeochemical process models to simulate the effect of grass-legume mixtures in relation to changing fertiliser application rates and the legume fraction within the sward. General response patterns in the models were then compared to a comprehensive experimental dataset which included measurements of biomass yields (Nyfeler et al., 2009), BNF and uptake of N from the soil (Nyfeler et al., 2011) from manipulated legume-grass fractions and rates of N fertiliser. Of particular interest was how well the two models simulated BNF and N yield, since these are critical factors in determining the potential benefits of grass-legume mixtures in relation to legume fraction and fertilizer N input.

2. Materials and methods

2.1. Experiment summary (following Nyfeler et al., 2009, 2011)

Specific details of the experimental data used here can be found in Nyfeler et al. (2009, 2011). In summary, the study aimed to quantify the changes in mineral N uptake, BNF and biomass production as affected by varying N fertiliser application rates and legume fraction in the sward. The experimental site was located near Zurich, Switzerland and the experimental design consisted of monocultures and sown combinations of two temperate C3 grass species, *Lolium perenne* L. and *Dactylis glomerata* L., and/or two legume species, *Trifolium repens* L. and *Trifolium pratense* L. (see Nyfeler et al., 2009). Replicate plots were sown in August 2002 and fertilised with N at rates (F), of 50, 150 or 450 kg N ha⁻¹ yr⁻¹, between 2003 and 2005. Fertiliser, applied in the form of ammonium nitrate (AN), was enriched with ¹⁵N to enable measuring BNF by isotope dilution (Nyfeler et al., 2011). Applications of fertilizer were made in April, May, June, August and September and followed by

biomass harvest approximately 30 days after each fertilizer amendment. After harvest, dry matter yields of each species in the sward were determined and an analysis of the ¹⁵N and N content was made.

2.2. Model descriptions

2.2.1. APSIM

APSIM (v7.8 r3972, Holzworth et al., 2014) is a process-oriented simulation framework comprising many task-oriented modules. Soil water, solute movement and below-ground competition for resources was simulated with SWIM3 (Huth et al., 2012). Soil organic matter and nitrogen transformations were simulated with Soil N as described by Probert et al. (1998) with more recent improvements described by Thorburn et al. (2010) and Vogeler et al. (2010). The Micromet module (Snow and Huth, 2004) dealt with above-ground competition between species. The pasture was simulated using one instance each of AgPasture (Li et al., 2011b, with recent additions to model reallocation of N reserves, for ryegrass and white clover (Vogeler and Cichota, 2016).

Nitrogen fixation in the legumes was calculated using a general linear function defined by two user-specified parameters. The first parameter was an obligate fixation which was set at a fixed fraction of plant N demand, and that amount of N was always symbiotically fixed (thus sparing demands on the soil mineral N) regardless of the mineral N available in the root zone. The second parameter was the maximum fraction of plant N demand that could possibly be supplied by N fixation. There was no direct account taken of the metabolic costs of symbiotic N fixation to the plant, but when mineral N was low in the soil and the maximum symbiotic fixation was less than unity there was a growth penalty arising from there being insufficient N.

2.2.2. DayCent

DayCent is a daily time-step, process-based model, that has been extensively used to replicate productivity and N₂O emissions from grassland ecosystems (Zimmermann et al., 2018; Senapati et al., 2016; Henderson et al., 2015; Fitton et al., 2014; Chamberlain et al., 2011). The model simulates the flows of C and N between the atmosphere, soil and vegetation and has evolved from the Century Soil Organic Matter Model (Del Grosso et al., 2005, 2010; Parton et al., 1998). Plant production is simulated as a function of solar radiation, available soil water and soil N. Plant residues and above- and below-ground organic material from animal excreta are separately partitioned into structural and metabolic pools, defined as a function of a ratio of lignin content to N. Organic nitrogen flow between pools follows that of C, via C:N ratios, which vary in the metabolic pools depending on the N content of plant residues, but is fixed for the structural pools. The N sub-model also estimates emissions of N₂O based on nitrification and denitrification.

As with other biogeochemical models, DayCent does not allow users to simulate multiple coexisting species. However, for each individual plant type simulated, including C3 grasses, legumes and crops, DayCent allows for BNF via the SNFXMX crop parameter. This parameter represents the maximum amount of N fixed per gram of C fixed via net primary production and only occurs if there is insufficient mineral N within the soil. As the model structure is sufficiently flexible i.e. it allows users to easily manipulate different input parameters. Therefore, not only can timing of management events be easily changed, but it also allows users to tailor different crop input parameters, as required here.

2.3. Modelling protocol

2.3.1. General modelling protocol

DayCent and APSIM are biogeochemical models that have some process descriptions in common but separate evolutionary histories. This includes a difference in the level of complexity represented in the simulation chain particularly for grassland systems.

Details on how each model implemented the varying legume fractions are given in the following sections. However, for consistency

Table 1

Soil properties of the Chamau (FLUXNET site ID: CH-CHA) experimental site provided to modellers (after Roth, 2006; Imer et al., 2013 and Merbold et al., 2014).

	0-250 mm	250-500 mm	500-750 mm	> 750 mm
Sand (%)	36	32	69	92
Silt (%)	45	42	21	6
Clay (%)	19	26	10	2
Bulk density (g cm ⁻³)	1.1	1.5	1.6	1.2
Saturated water content (m ³ m ⁻³)	0.56	0.41	0.39	0.52
Field capacity (m ³ m ⁻³)	0.47	0.37	0.34	0.20
Permanent wilting point (m ³ m ⁻³)	0.17	0.17	0.12	0.07
K _s (mm day ⁻¹)	1000	1000	1000	1000
Total organic C (%)	2.82	0.81	0.40	0.21
Total organic N (%)	0.31	0.10	0.05	0.03
pH in water	5.3	5.3	5.5	6.7

modelling rules pertaining to the soil, climate and management were developed by combining calibrated versions of each model to the Chamau grassland site (Merbold et al., 2014; Ehrhardt et al., 2018) with the grass-legume mixtures experimental design (Nyfeler et al., 2009, 2011). As neither model had a sufficiently robust mechanism for representing the sowing and germination process, a direct comparison with the data presented from the Nyfeler experimental site (most of which were from the two years after sowing) was unrealistic. Therefore, rather than replicating results from the necessarily time-limited, site-specific experiment, the modelling exercise focused on reproducing the general treatment response patterns of yield and BNF observed by Nyfeler et al. (2011, 2009). As the ultimate intent was to gain confidence in the model responses and then to apply this to the nearby Chamau grassland site (Merbold et al., 2014), where a GHG mitigation experiment using legumes is in progress (Fuchs et al., 2018a). Both models were, therefore, tested using the soil and long-term weather data (1980–2013) from Chamau grassland and management protocol from the Nyfeler site (Table 1). Yields and BNF over varying fertiliser rates and grass – legume fractions were simulated over this period and then compared with the corresponding observed dataset (Nyfeler et al., 2011).

The specific details on the timing and intensity of management events are described in Table 2, and for each model the same management schedule was adhered to between 1980 and 2013. This allowed for the long-term sward response to a change in management to be extracted. In addition, APSIM was also run with a zero-fertiliser rate to assist with the determination of the SNFXMX parameter for DayCent (see details later). Finally, as neither model has the capability to simulate the precise species or cultivars used in the experiment, general ryegrass and white clover parameterisations were used, and compared to the experimental data categorised as grass or legume only.

2.3.2. Grass-legume mixture model: APSIM

The grass-legume balance simulated by APSIM was an emergent property based on growth of the pasture components rather than being directly manipulated (as in the experiment) or input into the model (as

in DayCent). To achieve the varying ratios two steps were taken. First, in individual simulations, the species were initialised on 21-October-1980 at a range of ratios between 0 and 100% legume; the species were then re-initialised, at the same ratio, every third year on 21-October using an APSIM Manager component (Moore et al., 2014). Second, after each harvest event, the amount of each species harvested was calculated to achieve the desired legume fraction in the remaining un-harvested pasture. For example, if the target legume was 50% but the pre-harvest pasture contained 40% legume, then proportionately slightly more grass was harvested than legume to achieve the desired 50% ratio post-harvest.

In between the interventions described above, the grass-legume ratios were free to vary as a function of the normal competition processes and at times diverged from the target legume content. The data from harvests where the fraction of legume in the pasture deviated from the target legume content by more than 15 percentage points was excluded from the analyses. For the analyses involving annual values, if any harvest in a year was rejected then the whole year of simulated results was discarded. The percentage of rejected simulation years varied depending on the conditions (e.g. attempting to maintain a high clover content while also applying large amounts of fertiliser) but averaged about 35% and this was compensated for by running more increments of target clover content than was done for DayCent. Visual examination of the simulation results suggested that discarding this data did not affect the findings. It was performed so that legume content could be analysed as a categorical variable and to facilitate comparison with experimental data and DayCent. Specific details on the data analysis undertaken prior to discarding some APSIM data is detailed in the supplementary information (S.I.a).

2.3.3. Calculation of SNFXMX-L and use in DayCent

DayCent can only produce simulations for a single species and while the maximum N fixation can be modified, via the SNFXMX parameter, the value of this input, expressed as g BNF-N/g C NPP, is user defined rather than being an emergent property. As BNF varies with a changing legume fraction, L, it is sensible to assume that the value of SNFXMX at each fraction i.e. SNFXMX-L, would also change according to the clover fraction. APSIM, which simulates BNF as an emergent property, was therefore used to provide an estimate SNFXMX-L as a function of clover fraction. Model simulations were initiated as described in Sections 2.3.1 and 2.3.2 but also included simulations with a zero-fertiliser application. For each fertiliser application rate, the grams of N fixed per gram of C fixed via NPP, i.e. APSIM derived SNFXMX, between 1980 and 2013 were plotted against the legume fraction, L. After this, the individual harvest values of SNFXMX-L were binned into increments of 0.05 legume fraction (L) and a second-order polynomial equation with zero intercept being fitted to the maximum value in each bin. The resulting equation was used to calculate the value of SNFXMX for DayCent for each value of L. Within DayCent, for each legume fraction the SNFXMX value was adjusted accordingly, the remaining input parameters were left unchanged.

Although the SNFXMX parameter, described above, can be adjusted for each level of L (i.e. legume fraction from 0 to 1), this parameter represents only the maximum rate at which plant BNF can occur. The actual fixation will be generally lower as in DayCent the plants consider soil N uptake before BNF is calculated. As the plant input parameters

Table 2

Grassland management information used by both single and multispecies models.

Fertiliser application rates	0 kg N ha ⁻¹ yr ⁻¹ (APSIM only, for SNFXMX-L estimation) 50 kg N ha ⁻¹ yr ⁻¹ : in 5 equal splits 150 kg N ha ⁻¹ yr ⁻¹ : in 5 equal splits 450 kg N ha ⁻¹ yr ⁻¹ : in 5 equal splits
Fertiliser application dates	15 th April, 25 th May, 25 th June, 4 th August and 15 th September
Harvest dates	20 th May, 20 th June, 30 th July, 10 th September and 20 th October
Legume fraction	0.0, 0.05, 0.10, ... 0.95, 1.00

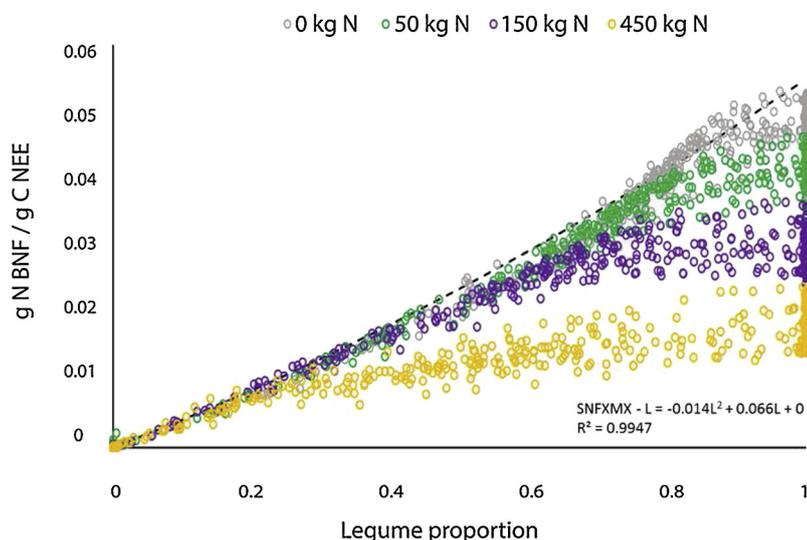


Fig. 1. The APSIM-predicted grams of nitrogen fixed for every gram of carbon fixed net primary production for four fertiliser application rates (see the key) and eleven legume fractions (L) within the sward. The dashed line indicates the fitted values (see equation) of SNFXMX-L. Model outputs are based on long term simulations (1980–2010) from the APSIM model.

represent a single vegetation type to reflect the diversity of species within the sward, two parallel simulations were made; one each of C3 grass and legume monocultures each with the value of SNFXMX to the corresponding legume fraction, L. Finally, the contribution of each plant type to the total yield and harvested plant N, was calculated based on the weighted average of each output with the weighting factor based on the fraction of legume (L) or C3 grass (1-L).

2.4. Calculations of yields, overyielding and transgressive overyielding

Our calculations of overyielding and transgressive overyielding were applied in a slightly different approach than in Nyfeler et al. (2009) which used the value of L from the prior year as the independent variable. Here we used L from the current year as neither APSIM nor DayCent included the sowing effects that were a key part of the year effect in Nyfeler et al. (2009). Neither could wither model effectively distinguish between the two grass and two clover types so, for comparison, when calculating biomass yields the observed data was treated as either as legume or grass.

Overyielding (O) was defined as being present when biomass production of a sward with multiple species has a higher productivity than would be expected if the yield was simply the weighted average of the two monocultures of the constituent species. Transgressive overyielding (T) was present when the biomass production of the mixed-species sward was greater than the productivity of the highest yielding monoculture (Schmid et al., 2008; Trenbath, 1974). We defined O_F as the maximum amount of overyielding at any fertiliser rate (F) and L_O as the value of L at which O_F occurs. Equivalent values for transgressive overyielding, T_F and L_T , were also determined. These quantities were found individually for each level of F by the procedure described below.

- 1 The median of the yield (kg DM ha^{-1}) in each 5% bin of L was found and a quadratic equation fitted to the medians. The medians were used because there was significant variation in the values of yield data with respect to L. The quadratic equation had the form:

$$Y(L) = aL^2 + bL + c \quad (1)$$

where Y was the fitted yield and a, b and c are fitted parameters and so that:

$$Y_0 = Y(L = 0) = c, \text{ and } Y_1 = Y(L = 1) = a + b + c \quad (2), (3)$$

- 2 The transgressive overyield (T_F , kg DM ha^{-1}) was the difference between $Y(L)$ at its maximum value and the largest of Y_0 or Y_1 ; this occurred by definition at L_T , where the first derivative of $Y(L)$ is

zero. Therefore,

$$dY(L)/dL = 2aL + b \text{ so that } L_T = -b/2a \quad (4)$$

$$T_F = aL_T^2 + bL_T + c - \text{Max}(Y_0, Y_1) \quad (5)$$

- 3 The overyield (kg DM ha^{-1}) for any fertiliser level (O_F) was the maximum difference between the mixing ratio yield of Y_0 and Y_1 (i.e. the straight line from Y_0 to Y_1). O_F and L_O were found by subtracting the mixing ratio (Y_{MR}) from Y and finding where the derivative equals zero. Therefore:

$$Y_{MR} = Y_0 + L(Y_1 - Y_0) \quad (6)$$

$$d(Y - Y_{MR})/dL = d(aL^2 + bL + c - Y_0 - L(Y_1 - Y_0)) / dL = 2aL + b - Y_1 - Y_0, \quad (7)$$

$$L_O = (Y_0 + Y_1 - b)/2a \text{ and } O_F = aL_O^2 + bL_O + c - Y_0 - L_O(Y_1 - Y_0) \quad (8)$$

The above equations were implemented in Microsoft Excel and evaluated for each level of F.

Confidence intervals of modelled overyielding estimates above were determined by using a bootstrapping analysis (Lee et al., 2017). Here for each model dataset and separately for each 5% increment data was sampled with replacement 10,000 times. At each level, L, the mean, upper and lower confidence intervals were then calculated from the derived datasets. By re-fitting the quadratic functions as described above to the maximal and minimal values across the ranges of L, overyielding and transgressive over-yielding were calculated to give a confidence interval for modelled values. There were insufficient data points in the experimental data for this procedure, so this analysis was applied only to the model outputs.

3. Results

3.1. APSIM-derived SNFXMX-L estimations

For each N fertiliser rate, the ratio of BNF (g N) and plant NPP (g C) of the whole sward i.e. grass and legume combined, increased as L increased (Fig. 1). Additionally, at any value of L, as N application increased there was a decrease in the ratio of BNF, this however was less discernible at lower values of L. This was due to the increased availability of mineral N within the soil for use by the legume, which then suppresses symbiotic N fixation. A second order polynomial equation with zero intercept was fitted to the maximum values of BNF across all levels of N, including simulations where no fertiliser was applied. The

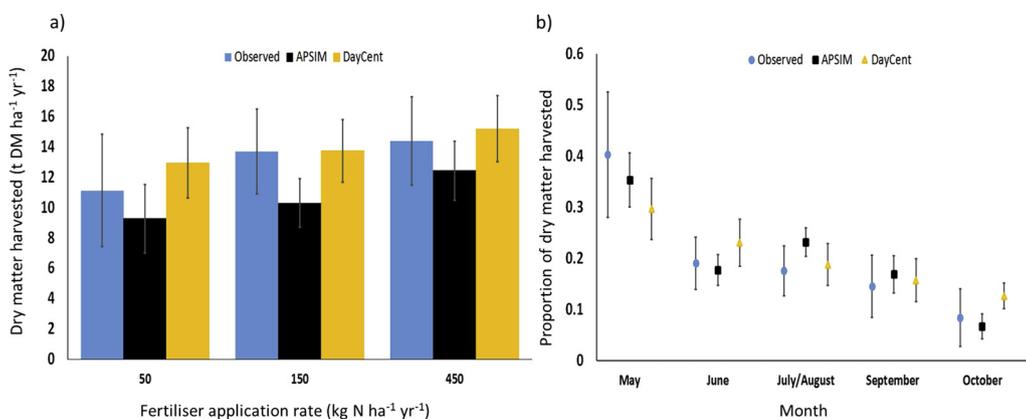


Fig. 2. (a) The observed and predicted annual dry matter harvested (t DM ha⁻¹ yr⁻¹) averaged across all experimental plots as affected by N application rate (kg N ha⁻¹ yr⁻¹), (b) the observed and predicted dry matter (t DM ha⁻¹ yr⁻¹) for each month of harvest throughout the year for all fertiliser levels. For DayCent the dry matter harvested represents the weighted mean of the parallel grass and legume simulations. Whiskers represent the standard deviation in the range of values measured or simulated. For both APSIM and DayCent, model outputs are calculated based on long term results (1980–2010).

resulting equation (Fig. 1) was used then to calculate the SNXFMX-L. These values were then used in DayCent for the parallel model runs of grass and legume species at each legume fraction, L.

3.2. Comparison between the observed and multiple and single species model outputs

Modelled outputs of dry matter yields, total above ground plant N and BNF were compared with the observed values across the range of F and L. APSIM tended to underestimate observed average annual yields, particularly when 150 kg N ha⁻¹ was applied, although the differences were not statistically significant (Fig. 2a). For DayCent, at the lowest N application rate, yields were overestimated but otherwise there was a good agreement with the measurements. Both models showed a greater yield response when the N application increased from 150 to 450 kg N ha⁻¹ than seen in the measured data (Fig. 2a) but there were no statistically-significant differences between the data sources. The highest yields were always those taken after the first harvest in May, and lowest yields were taken at the end of the growing season in October (Fig. 2b). Across all harvested data from the observed values and DayCent datasets, the fraction of harvested material decreased gradually from May to October. For APSIM, though, a higher fraction of biomass yield was harvested in July compared to June or October (Fig. 2 b) suggesting some seasonal influence however there was no statistically-significant differences.

Both the observed and simulated grass yields also changed in relation to the legume fraction, L, of the sward (Fig. 3). Across each of the three datasets, yields, particularly at low values of L, tended to increase with increasing fertiliser rates. However, where the swards were entirely comprised of legumes the yields did not vary significantly across the different fertiliser rates.

While trends in APSIM and the observed yields are based on legume fractions that vary within each bin (Fig. 3), the DayCent results had a degree of rigidity in the simulated yields. More specifically, for each value of L, the variability in predicted yields were due to inter-annual variation driven by climate variation rather than a variation in legume fraction (Fig. 3). This was because although the SNXFMX parameter is user defined the fraction of N fixed per gram of C remains fixed throughout the year and only adjusted by modelled NPP. Consequently, under the single runs of grass and legume swards as L increased modelled yields tended to consistently reach the maximal value (S.I.3, S.I.4). Therefore, the distinctive curve shape of the sward yields (Fig. 3) to a changing legume fraction was the result of combining the weighted average of parallel runs.

For all data sources, at F = 150 kg N ha⁻¹, as L initially increased, the amount of N harvested increased (Fig. 4a) until a plateau was reached at L ~ 0.5. However, neither model replicated the distinct peak observed in the experimental data (Fig. 4a). APSIM outputs were compared to the experimental non-BNF-N (this output is not obtainable

from DayCent) in Fig. 4b. The trends were consistent, in that, for both data sources there was a gradual decline in non-BNF-N as L increased.

A more interesting comparison is the fraction of total N originating from BNF in relation to L as affected by F. For both datasets there was a strong relationship between the fraction of harvested N derived from BNF and L (Fig. 5) including a decline at high values of L. Biophysically, the decline in the proportion of N from BNF with increasing L could plausibly be explained by reduced competition for soil mineral N from the grass component of the sward with increasing L resulting in increased uptake of soil N by the legumes and from there to reduced BNF. In addition, as F increased the fraction of BNF-N decreased, which is due to the increased amount of mineral N being available in the soil.

3.3. Overyielding and transgressive overyielding

For each dataset, and regardless of F, the point at which maximum overyielding tended to occur was when L ~ 0.5 (Table 3). The legume fraction at which the maximum transgressive overyielding occurred was also dependent on F. All data sources showed that the legume content for the greatest transgressive overyielding i.e. the mixture with the highest yield decreased with increasing fertiliser application.

4. Discussion

Regardless of ecosystem structure, a model should exhibit a sensitivity to changes in management particularly, fertiliser application rates. When nitrogen fertilisers are applied directly to the soil, nitrogen becomes readily available for plant uptake, and most modelling or experimental studies have shown a positive relationship between pure grass yields and N application rates over the range of rates used in this study (Whitehead, 2000; Moir et al., 2012; Fitton et al., 2014, 2017). A more difficult and complex relationship to simulate, however, is the amount of BNF and the presence of legumes in the sward at varying fractions.

APSIM is a biogeochemical model that can simulate productivity and greenhouse gas emissions which characterise most grassland ecosystems (Snow et al., 2014). The model uses a scheme inspired by DayCent to calculate the fraction of total nitrification and denitrification that is emitted as N₂O (Thorburn et al., 2010). Beyond that, both models have divergent histories and process representations (Parton et al., 1998; Holzworth et al., 2014). A particular strength of APSIM is an in-built ability to model competition between grasses and legumes and therefore the flow-on effects of that competition on BNF. One example of this is that grasses can out-compete legumes for soil mineral N, if sufficient levels are available, because of the differences in their root morphology, this means that the legumes obtain less soil-derived N and increase their BNF. Details on modifications made to the model for use in this type of study are described in Section 2.3.2.

For single species models, previous modelling studies such as Li et al

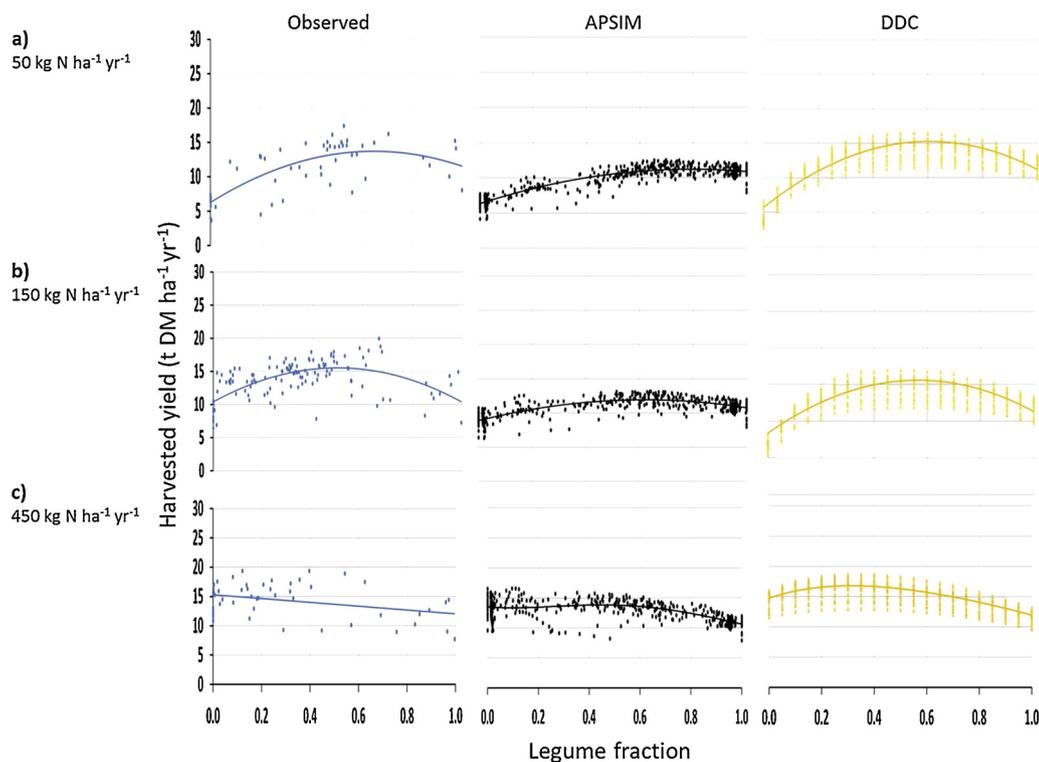


Fig. 3. The observed and dry matter harvested ($t DM ha^{-1} yr^{-1}$) in relation to an incremental increase in the legume fraction and an increasing N application rate ($kg N ha^{-1} yr^{-1}$) from the experimental plot, APSIM and DayCent. For DayCent the dry matter harvested represents the weighted mean of the parallel grass and legume simulations. For both APSIM and DayCent, model outputs are based on long term simulations (1980–2010).

(2011a), focused on modelling legumes incorporated into grass swards, and model success was limited to a site level calibration. Much of this has been at the expense of exploring the challenges to single species models in simulating complex interactions such as differences in growth controls and N content of biomass (Nyfeler et al., 2009, 2011; Hofer et al., 2017, 2016). DayCent, which has an established track record in grasslands studies, allowed for such challenges to be investigated due to

the ease at which crop input parameters could be modified. Therefore, the resulting novel approach adopted here, i.e. using the APSIM-derived BNF outputs as an input for DayCent and mixing the weighted contribution of the parallel runs of grass and legume *post hoc*, allowed for a more realistic growth pattern and plant N representation to be achieved. There are, however, several caveats to the approach. These include, for example that the simulated yields from DayCent do not

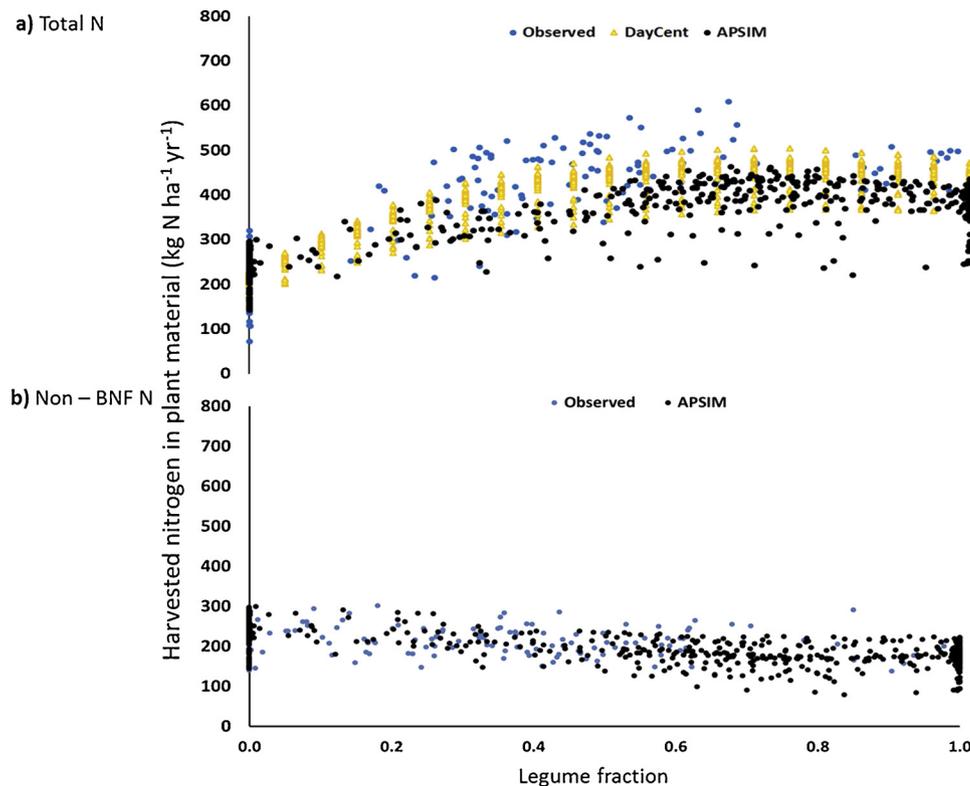


Fig. 4. a) The observed and predicted harvested nitrogen content in the plant material ($kg N ha^{-1} yr^{-1}$) across all experimental plots with an N application rate of $150 kg N ha^{-1} yr^{-1}$ plotted against an increasing legume fraction. Here for DayCent the harvested N represents the weighted mean of the parallel grass and legume simulations; b) The observed and predicted nitrogen content, due to non-symbiotic N fixation, of dry matter harvested ($kg N ha^{-1} yr^{-1}$) across all experimental plots with an N application rate of $150 kg N ha^{-1} yr^{-1}$ plotted against an increasing legume fraction. DayCent cannot provide estimates of non-BNF N. For both a) and b) model outputs are calculated based on long term simulations. (1980–2010).

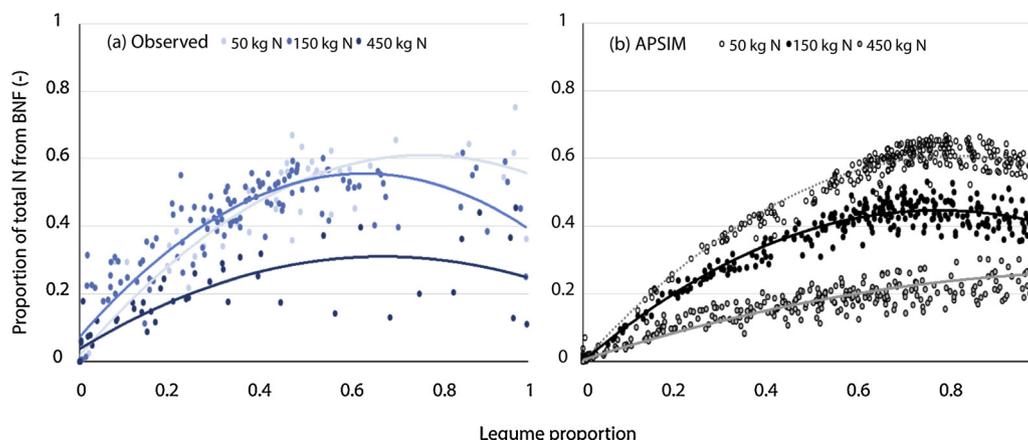


Fig. 5. The observed (a) and APSIM-predicted (b) fraction of total N harvested originating from biological N fixation (BNF) as affected by legume fraction and fertiliser rate. DayCent cannot provide estimates of the fraction of N from BNF. Model outputs are based on long term simulations (1980–2010).

Table 3

Estimates of the maximum clover fraction at which (a) overyielding and (b) transgressive overyielding occurs as determined from observed, APSIM, and DayCent data. Values here are estimated based a polynomial fit between the dry matter harvested and the legume fraction.

	Observed	APSIM	DayCent
Overyielding			
50 kg N	0.5	0.5 (0.01)	0.5 (0.01)
150 kg N	0.5	0.4 (0.03)	0.5 (0.01)
450 kg N	0.5	0.5 (0.03)	0.5 (0.01)
Transgressive overyielding			
50 kg N	0.6	0.6 (0.05)	0.6 (0.02)
150 kg N	0.5	0.4 (0.03)	0.5 (0.01)
450 kg N	0.3	0.3 (0.03)	0.3 (0.01)

represent the inter-annual variability of the legume fraction within the sward as demonstrated in the observed and APSIM datasets. The potential overestimation of N uptake across the year could therefore have resulted in higher yields being simulated leading to an overstatement of the net benefits of grass – legume mixtures, such as reduction in N_2O emissions and reduction in fertiliser dependence.

Another potential limitation to this approach was the applicability of the methodology described here to beyond a site level application. Therefore, we repeated the simulations used to derive SNFXMX-L for the five diverse soil-climate combinations used in the grassland sites reported by Ehrhardt et al. (2018) and Sándor et al. (2018). These tests (Fuchs, 2018b) demonstrated that for a C3 grass/legume mixture, the APSIM derived SNFXMX values did not vary significantly between quite divergent sites. Suggesting a universality to the estimation of SNFXMX-L and therefore to the methodology developed here. As the dependency of DayCent on APSIM, in the approach adopted here, was primarily related to a requirement to initiate the model with a reasonable estimate of the maximum rate of N fixation across a range of legume fraction which is unavailable in the literature. Like other crop parameters, such as temperature responses or productivity, once available, generic estimates of each input can be used for upscaling model runs, much like in the approach adopted in Fitton et al (2014).

Going forward, despite apparent advantages of multiple species like APSIM models to different. A recent study by Ehrhardt et al. (2018) demonstrated that a model ensemble consistently provided a more accurate representation of the N_2O emissions and productivity from a range of experimental sites than any single model. Consequently, future modelling protocols may increasingly adopt this ensemble approach for emission simulation studies. DayCent is widely used model that has been successfully tested against N_2O emissions and productivity in a range of different regions and ecosystem types (Parton et al., 1998; Del

Grosso et al., 2010 and Fitton et al., 2014). It is therefore well placed for use in ensemble modelling. Moreover, the successful application of multiple-model simulations used here allowed for an investigation as to if the presence of two or more species may lead to productivity gains (De Deyn et al., 2012; Finn et al., 2013). This includes the provision of supporting evidence of overyielding in grassland ecosystems as described in Balvanera et al. (2006) and Cardinale et al. (2007). Here, each of the data sources agreed that overyielding occurs when there is a 50:50 species mixture. However, with regards to transgressive overyielding the results were less clear, which is in line with the current literature (Cardinale et al., 2006; Schmid et al., 2008; Kirwin et al., 2009; Nyfeler et al., 2009). Both, the observed and APSIM values indicated that a grass-legume mixture has the potential to be more productive than either monoculture. This was clearly reflected in the experimental datasets (Nyfeler et al., 2009) and over a wide range of growth conditions (Finn et al., 2013; Brophy et al., 2017; Suter et al., 2015).

5. Conclusions and further work

Using an existing experimental dataset, a grass-legume model, APSIM, was used to provide a BNF parameter for the single species model DayCent. This approach subsequently allowed for an understanding of the different methodological approaches that could be adopted to reconstruct the relatively complex interactions in grass-legume swards. Finally, if trends in for example biomass yields could be replicated, the methodology applied here could be used in future modelling studies to evaluate the potential advantages of grass-legume swards for meeting production and environmental targets.

The methodology adopted here describes a novel approach to using DayCent, a single species model, to predict biomass yields, N uptake and BNF from mixed swards. While both models suffered from some limitations, for example in APSIM the user could not directly control the clover content. Or in DayCent, the methodology adopted here required two simulations and post-processing of results which has the potential to become cumbersome to use in large spatially disaggregated simulations. Our work suggests that single species models, such as DayCent, should not be used for grass-legume mixtures beyond about 30% legume fraction unless used with a scheme such as that described here. As such, these single-species models, when used in a straightforward mode beyond this limit may be unsuitable for N_2O mitigation studies that consider the role of legumes. If biogeochemical process models, such as DayCent, are to be used beyond these limits, they must evolve to encompass the key processes, such as species interactions and intra-annual variability of the legume fraction over the year on the outputs of interest. This must be achieved without becoming so complicated that

they become intractable. It is also important that further experimental work, much in line with the experiment used here, are carried out to help inform and critically evaluate models in current usage.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:<https://doi.org/10.1016/j.eja.2019.03.008>.

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