

Appendix C. Model description

CENTURY model

General settings

We reconstructed the CENTURY model based on the equations published in literature (Parton et al. 1998; Parton et al. 1987; Parton et al. 1993; Parton et al. 1988) and source code (Metherell et al. 1993). The model consists of different processes, e.g. plant production, SOM dynamics, hydrology. We used the equations and parameter values of CENTURY version 4 (Metherell et al. 1993) unless specified. When a parameter value is specific for different vegetation types, we took those for temperate grasslands ('TG'). The original CENTURY computes SOM dynamics weekly and plant production monthly, whereas we simulate them on a daily basis. Accordingly, parameter values with weekly and monthly rates were converted to daily rates (with a factor 1/7 and 1/30, respectively).

CENTURY uses multiple soil layers with constant depths. We set three soil layers of 20 cm (topsoil), 50 cm, and 50 cm depth. We assumed that all soil organic matter exist in the topsoil layer. Water and dissolved N moves between soil layers. We assumed that all roots are distributed in the topsoil layer. This means that plant took up nutrients only from the topsoil layer, and drought stress on plant production was controlled by moisture content of the topsoil. Mineral N pool was split into ammonium and nitrate pools, as in the daily version of CENTURY, DAYCENT (Del Grosso et al. 2002). With these pools, we also simulated nitrification and denitrification processes following the DAYCENT model.

Below is the brief explanation of each sub-module of CENTURY model, as well as modifications of equations and parameter values made for this study. For more detailed description of CENTURY model, see original literature (Parton et al. 1998; Parton et al. 1987; Parton et al. 1993; Parton et al. 1988).

Plant production

Potential above-ground plant growth is calculated by multiplying the vegetation-specific maximum growth rate with three controlling factors; soil temperature, soil moisture, and self-shading. In our study, the maximum growth rate was obtained by the optimization procedure (see section 'Parameter optimization'). Allocation of biomass to shoot and root was set to be constant and calculated as a function of typical annual precipitation of the study sites, i.e. 80 cm yr⁻¹. To prevent unrealistically fast growth in the first years when the simulation starts from bare soils, we added an equation to restrict plant production relative to their current biomass, with the maximum relative growth rate (g g⁻¹ d⁻¹). We used the mean value of maximum relative growth rate of 105 UK plants on a weekly basis, 1.2 g g⁻¹ week⁻¹ (Dawson et al. 2011), converted to a daily value with an assumption of exponential rather than arithmetic growth (i.e. 0.12 g g⁻¹ d⁻¹).

Actual plant growth is controlled by the availability of N. C:N ratio of shoots and roots change dynamically within the minimum and maximum C:N ratios, depending on available mineral N in soil and from symbiotic N₂ fixation. The minimum and

maximum C:N ratios of shoots were calculated as a function of shoot biomass. Since the minimum and maximum C:N ratios of shoots in CENTURY ver.4 for temperate grasslands (maximum C:N ratio 90-95, minimum C:N ratio 30-35) were much higher than the range observed in our field study in Dutch dune ecosystems (Fujita et al. 2013b), we adapted these parameters to the empirical values in our dataset: maximum C:N ratio 36 (50th percentile) – 59 (90th percentile); minimum C:N ratio 25 (10th percentile) – 36 (50th percentile).

Available mineral N in soil for plant uptake, N_{ava} , is restricted by root biomass as:

$$N_{ava} = mineralN \cdot (1 - riint \cdot \exp(-rictrl \cdot C_R \cdot ratbioC)) \quad (C.1)$$

where $mineralN$ is mineral N (nitrate plus ammonium) in topsoil ($gN\ m^{-2}$), C_R is the amount of C in root ($gC\ m^{-2}$), $riint$ and $rictrl$ are the coefficient values to determine the shape of root-size effect on N availability. The default values of $riint$ and $rictrl$ in CENTURY ver.4 are 0.8 and 0.015, respectively. To restrict the nutrient uptake when root biomass is very small in the beginning of succession, we changed the $riint$ value from 0.8 to 0.99 (i.e. 1% of nutrient is available for roots when there is no root, instead of 20 %). $rictrl$ value was obtained by the optimization procedure (see section ‘Parameter optimization’).

Symbiotic N fixation is assumed to occur when soil mineral N is not sufficient to satisfy the plant N demand having taken into account all the other factors which limit growth of plant (e.g. temperature, moisture). Symbiotic N fixation can occur up to a maximum level of N fixed per C fixed, with a N:C ratio specific to each plant type ($snfxmx$). Since CENTURY model assumes monoculture crop systems, the value of $snfxmx$ is either $0\ gN\ gC^{-1}$ (for non-N-fixers) or $0.0375\ gN\ gC^{-1}$ (for legume crops such as alfalfa). In natural ecosystems, however, symbiotic N-fixers (predominantly legume species) are ubiquitous and they typically occupy a few percent of the total cover. Thus, we introduced a new parameter, $nfxrat$ (fraction between 0 and 1), to include the proportion of N fixers in plant production.

The maximum symbiotic N fixation ($nfixmx$, $gN\ m^{-2}\ d^{-1}$) is computed as:

$$nfixmx = P_P \cdot snfxmx \cdot nfxrat \quad (C.2)$$

We used different values of $nfxrat$ for the three chronosequences based on measured percentages of plant species associated with N fixers (see section 2.6). If available mineral N plus maximum symbiotic N fixation is enough to support the potential production with the maximum C:N ratio (i.e. N-poor biomass), actual production equals to potential production. If not, actual production is reduced.

Death of shoots is calculated as a function of soil moisture and shading effects. In addition, in the beginning of winter, 95% of living shoots die. Death of roots is calculated as a function of soil moisture and soil temperature. Dead shoots flow into standing dead pool, and then flow into surface litter pools (i.e. surface metabolic and surface structural) with a function of lignin:N ratio. Dead roots flow into root litter pools (i.e. belowground structural and belowground metabolic) with a function of lignin:N ratio.

Soil organic matter dynamics

C in soils is divided into 8 pools (surface structural and metabolic, belowground structural and metabolic, surface microbe, active, slow, passive). C in each pool is decomposed with pool-specific maximum decomposition rates, multiplied with reduction factors by soil moisture and soil temperature. We optimized the maximum decomposition rate of the slow pool (see section 'Parameter optimization'). The decomposed C flows into other pools, and some of the flows were influenced by lignin content and soil texture.

N dynamics

Soil organic N flows are coupled with C flows. The outflow of N is proportional to that of C, whereas the inflow of N into a pool is the product of the C inflow into the pool and the N:C ratio of the pool. N:C ratios of soil pools varies, as N:C ratios of inflows change dynamically depending on N concentration of the plant residues (for surface microbe pool) or mineral N (for active, slow, and passive pools).

N is mineralised if in excess, and immobilized from mineral N pool if in shortage. When potential N mineralisation is negative (i.e. net N immobilization) and if the amount of ammonium concentration in soil is not enough to enable the immobilization, decomposition is inhibited.

Nitrification and denitrification are modelled according to the daily version of CENTURY, DAYCENT (Del Grosso et al. 2002), except for the pH-dependent terms of nitrification and denitrification. Since mineral N pool in the top soil is not separated into nitrate and ammonium (and therefore no preferential uptake of nitrate or ammonium by plants, no difference in leaching rates between nitrate and ammonium), the influence of the nitrification is restricted to the subsequent denitrification in our model. Note that, in our study sites, denitrification hardly occurs due to the prevailing dry conditions in the soil.

N leaching is computed as amount of mineral N (ammonium and nitrate) moving from the 3rd soil layer to the layer beneath. We did not use the soil texture effect on N leaching used in CENTURY ver.4, as it bases on empirical relationship which we could not check if it is applicable to our target ecosystem. Instead, transfer of mineral N in soil was simply calculated as the products of the water flows and the concentration of mineral N in the originating layer.

N input via atmospheric deposition (dry plus wet, as ammonium or as nitrate) was simply added to the ammonium pool and nitrate pool in the topsoil layer. The annual rate of N deposition was divided by 365 to get the daily rate of N deposition.

Non-symbiotic N fixation (i.e. N fixation by free-living microorganisms) is formulated either as a function of precipitation or as a function of N:P ratio in mineral pool in CENTURY ver. 4. Since the coefficient values of these functions in CENTURY were obtained by model tuning procedure (Parton et al. 1987) and therefore not underpinned by theoretical or empirical evidence, we assumed simply a constant rate of non-symbiotic N fixation all through the year. We used a the median

value of the study in temperate unfertilized grasslands (Reed et al. 2011), $0.57 \text{ gN m}^{-2} \text{ yr}^{-1}$. The fixed N is added to the ammonium pool of mineral N in the topsoil layer.

Hydrology

A simple hydrological model of CENTURY model (Parton et al. 1993) was used to simulate water flows between soil layers. Snow and liquid snow were omitted. Plant-related parameters (living biomass, standing dead materials, surface litter) were updated every month from the plant production module of the model. Equations of the hydrological module are fully described in Appendix B of Parton et al. (1993).

Parameter optimization

We optimized the following three model parameter values: the maximum above-ground plant growth per day under optimal condition ($\text{gC m}^{-2} \text{ d}^{-1}$), the parameter controlling the impact of root biomass on nutrient availability for plants, and decomposition rate of the slow pool of soil organic matter (fraction/day). The parameter values were optimized using least-square object functions of regression methods using the software 'UCODE' (Hill and Tiedeman 2007). The purpose of this procedure is to optimize these global (i.e. not site-specific) parameters so that the model outputs are roughly tuned to typical ranges in dune ecosystems. Because incorporating pH as a controlling factor for decomposition in dune soils is still difficult (unpublished data), we calibrated one model for both calcareous and acidic soils. Therefore, we used observed data of LD, averaged over calcareous and acidic sites together, but not that of NB which has calcareous sites only. The used observation data was soil C, soil N, and above-ground plant biomass at the peak season of five succession ages.

Model initial values

For all sites, we assumed that dune succession starts from bare sand. Although our measurements indicated that bare sand contains a little amount of soil C and N, we assumed in the model that the initial bare sand does not contain any C and N. Ignoring those initial amounts of C and N hardly affected the model outputs. Grain analysis of similar soils to NB and LD suggested that there are only ignorable amount of clay and silt in the soils in our plots: no clay or silt in west coast dunes similar to NB (Allen et al., 2014), and only $\sim 0.6\%$ clay and $\sim 1.7\%$ silt in the same dune areas as LD (Fujita et al., 2013a). For simplicity, we used the same proportion of clay, silt, and sand content for both sites as model inputs: 0% for clay, 5% for silt, and 95 % for sand. Parameters to determine soil water retention characteristics (i.e. water content at wilting point, 0.010, and at field capacity, 0.124) were calculated for pressure heads of -16000 cm and -100 cm, respectively, using soil physical parameters of typical Dutch sandy soils (Wösten et al. 2001).

Initial water content of three soil layers was obtained by running the hydrological model for 365 days prior to the start of the simulation date. Initial concentrations of mineral N (nitrate and ammonium) in the soil water were assumed to be zero.

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