

Original Article

A physiological and biophysical model of coppice willow (*Salix* spp.) production yields for the contiguous USA in current and future climate scenarios

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ABSTRACT

High-performance computing has facilitated development of biomass production models that capture the key mechanisms underlying production at high spatial and temporal resolution. Direct responses to increasing [CO₂] and temperature are important to long-lived emerging woody bioenergy crops. Fast-growing willow (*Salix* spp.) within short rotation coppice (SRC) has considerable potential as a renewable biomass source, but performance over wider environmental conditions and under climate change is uncertain. We extended the bioenergy crop modeling platform, BioCro, to SRC willow by adding coppicing and C3 photosynthesis subroutines, and modifying subroutines for perennation, allocation, morphology, phenology and development. Parameterization with measurements of leaf photosynthesis, allocation and phenology gave agreement of modeled with measured yield across 23 sites in Europe and North America. Predictions for the continental USA suggest yields of $\geq 17 \text{ Mg ha}^{-1} \text{ year}^{-1}$ in a 4 year rotation. Rising temperature decreased predicted yields, an effect partially ameliorated by rising [CO₂]. This model, based on over 100 equations describing the physiological and biophysical mechanisms underlying production, provides a new framework for utilizing mechanism of plant responses to the environment, including future climates. As an open-source tool, it is made available here as a community resource for further application, improvement and adaptation.

Key-words: BioCro; bioenergy; climate change; crop models; modeling; photosynthesis; poplar; WIMOVAC.

INTRODUCTION

Biofuels may provide a local and sustainable energy supply that reduces dependence on fossil fuels (Somerville *et al.* 2010). Given concerns over competition with food (Valentine *et al.* 2012), and impacts of direct and indirect

land use change on greenhouse gas (GHG) emissions (Anderson-Teixeira *et al.* 2009), perennial bioenergy feedstock grown on land unsuited to food crops has particular value. Cellulosic ethanol produced from perennial grasses and shrubs grown on marginal lands would reduce competition between food and fuel (Heaton *et al.* 2008; Somerville *et al.* 2010; Wang *et al.* 2010, 2012a), while delivering superior net GHG benefits to ethanol derived from food crops (Anderson-Teixeira *et al.* 2012). Woody species managed as short rotation coppice (SRC) have multiple advantages over first-generation annual biofuel crops. These include (1) enhanced biological diversity (Rowe *et al.* 2009); (2) greater carbon sequestration (Baum *et al.* 2009; Don *et al.* 2011); (3) reduced inputs of labor, pesticides and fertilizers (Hill *et al.* 2006); and (4) greater stability of biomass supply due to the longer harvest cycle and ability to store wood on the plant until needed.

Hybrid willows are among the most widely cultivated hardwood species due to their rapid growth, ease of planting and rapid resprouting after coppicing, as well as adaptation to diverse soil types (Mitchell *et al.* 1999; Mead 2005). Yields depend on climate, soil type, management and genotype. These crops are typically grown on a 3–5 year rotation and remain viable for 15–30 years (Aylott *et al.* 2008). With such a long cropping cycle, a crop will likely experience significant increases in atmospheric [CO₂] and annual average temperature between the time it is planted and the end of its productive life (IPCC 2013). A review of yields from previously published field trials in the Biofuel Ecophysiological Traits and Yield Database (BETYdb, LeBauer *et al.* 2010) showed a mean annual dry mass yield of SRC willow of 7.3 Mg ha^{-1} ($n = 349$, $\text{SD} = 4.5$) in field plantations across Europe ($n = 216$, Nordh 2004; Aylott *et al.* 2008) and the USA ($n = 68$, Randall *et al.* 2010; Volk *et al.* 2011). However, this reflects where the crop has been and much higher yields should be expected going forward. New triploid hybrids have produced up to $17 \text{ Mg ha}^{-1} \text{ year}^{-1}$ in trials in northern New York State (Serapiglia *et al.* 2014). Actual yield data are critical to the development of the second-generation bioenergy industry but at present only represent a tiny fraction of sites where the crop could be grown, and do not inform us of future yields under atmospheric and climatic change. Model

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prediction of willow productivity over large spatial scales and under elevated $[\text{CO}_2]$ and temperature fills an important gap in understanding of its potential as a bioenergy crop, now and into the future.

Where yield observations provide sufficient coverage in space and time, as is the case for major food crops (Rosenzweig *et al.* 2014), empirical statistical models provide a useful tool for regional yield predictions. However, this approach is not applicable to predicting willow yields for the USA, where production trials have been too limited in number and geographic range to allow effective empirical models. Furthermore, no large-scale experiments have tested the impacts of the increases in temperature and $[\text{CO}_2]$ expected to occur over the next few decades. In this context, mechanistic physiologically based models are more appropriate than statistical models for predicting yields, since mechanism provides a principled method of projecting outside of the observation domain of observation. For this reason, the development and parameterization of mechanistic models is critical to predicting carbon assimilation, growth and yield at spatial scales ranging from individual fields to regions for emerging bioenergy crops. This is important in evaluating the best choice of crop(s) for developing bioenergy projects for different locations and constraints. Further, C_3 plants respond directly to rising atmospheric $[\text{CO}_2]$, through its direct effects on photosynthesis and stomatal conductance. These effects and the interactive effects of rising $[\text{CO}_2]$ and temperature are well defined mathematically at the level of leaf processes (Long *et al.* 2004). Mechanistic models that capture these effects are therefore particularly valuable in projecting future productivity under conditions of atmospheric and temperature change that will influence the productivity of these systems over the decadal time scale of a willow coppice planting.

Empirical models using partial least squares regression between yields with multiple driving factors including soil chemical composition, diurnal temperature range and seasonal climatic variations have been shown effective for simulating willow yield in Europe (Aylott *et al.* 2008). Such models are appealing due to their simplicity but their parsimonious nature does not allow detailed description of the processes driving photosynthesis and resource use, which in turn obscure linkages among climate, soil and productivity, and projection beyond experimental experience. To evaluate and better understand the physiological, biophysical and physical processes, as well as the impacts of climatic and atmospheric change, a process-based model for plant growth which includes the underlying biochemistry and biophysics, canopy structure and dynamics, and allocation would be more appropriate.

Many process-based models provide sufficiently accurate predictions for a range of potential biofuel crops. For example, ForestGrowth-SRC is a process-based model that accurately predicts observed willow yields (Tallis *et al.* 2013). However, comparing potential yields for different biofuel feedstocks predicted by different models conflates differences in species or genotype behaviour with differences in model structures and approaches. To parse the biological

effects of a particular crop from different approaches to simulating the agroecosystems as a whole, there is a need to develop a shared modeling framework that supports multiple crop species and functional types. The mechanistic modeling framework, BioCro, has proved effective in predicting yield and yield stability of switchgrass and *Miscanthus* in the USA (Miguez *et al.* 2009, 2012). Adding SRC willow to the BioCro modeling framework provides a consistent set of assumptions upon which yield potential among second-generation perennial bioenergy crops can be compared.

BioCro provides mechanistically rich crop growth models specific to individual species, developed from the principles of a generic mechanistically based model of plant growth and productivity, WIMOVAC. WIMOVAC encapsulates the key underlying biochemical, biophysical and canopy microclimate processes using hourly time steps (Humphries & Long 1995). This is the first use of BioCro to simulate the growth and production of coppiced trees/shrubs, or any C_3 crop. Our new willow model also provides one of the most mechanistically detailed growth and production models available for a woody species. It uses detailed hourly weather to predict photosynthesis, respiration, transpiration and microclimate throughout each day and soil properties to predict the dynamics and distribution of soil moisture across 10 layers. Growth, production and turnover of organs are predicted on a daily time step.

Although most trials and commercial production of shrubby willows in SRC have been in Western Europe, there is now considerable interest in the crop for the USA (Volk *et al.* 2006).

In this study, we use this model to predict production across the contiguous USA and how it may be affected by global change. The specific objectives were to (1) simulate SRC willow by developing coppicing, perennation, C_3 leaf photosynthesis, canopy CO_2 assimilation, allocation and phenology sub-models within BioCro; (2) validate model performance with observations from field trials across Europe and the North America, independent of the calibration data; and (3) upscale the model to provide high-resolution regional predictions for the USA under current and future elevated $[\text{CO}_2]$ and temperature.

MATERIALS AND METHODS

The structure and sub-models in BioCro have been described, in full, previously (Humphries & Long 1995; Miguez *et al.* 2009, 2012), so the following description focuses on the processes and parameters specific to adapting the model to SRC willow. However, the complete set of 106 equations from CO_2 uptake in different canopy layers and moisture uptake in different soil layers to the dynamics of partitioning resources is given in Supporting Information (Table S1), together with the definitions of terms and sources of parameters. The source code and data used to produce this analysis are available as an archive that includes climate, soil, and yield data, as well as the R package BioCro v.0.92 (Miguez *et al.* 2015), while the development version of BioCro is available publicly on GitHub (<http://github.com/>

ebimodeling/biocro). In brief, BioCro uses light, temperature, humidity and $[\text{CO}_2]$ to predict photosynthesis and respiration rates at hourly time steps in each canopy layer. Simultaneously, canopy transpiration and water extraction from different soil layers are predicted. Net carbon gain or loss over the day is partitioned between organs based on developmental stage and in turn determined by thermal time and by day length or temperature thresholds. These factors also determine leaf appearance and loss. Physical models of water movement combined with soil properties, and coupled with root distribution and growth are used to predict dynamic changes in soil water distribution. Similarly, biophysical models of microclimate coupled with the profile of leaf nitrogen content within the canopy are used to predict photosynthesis, transpiration and respiration in the different layers of the crop canopy. Leaves in each layer are treated as two dynamically changing populations of sunlit and shaded leaves for the purposes of computation of photosynthesis and transpiration.

Macroclimate and soil database

Climate data for the model validation sites (listed in Table 1) came from different sources. For four sites (Balbirnie, Trefeinon, Trumpington and Loyton Bampton) given in Aylott *et al.* (2008), hourly temperature, precipitation, photosynthetically active radiation (PAR), wind speed and relative humidity (RH) were obtained by personal communication and are now stored in the BioCro v0.92 package; for all the other sites, daily weather data were obtained from NARR (North American regional reanalysis climate database). Day of year, hour and latitude were used to determine the hourly solar declination and zenith angle (eqns 1–8 in Supporting Information Table S1). Hourly values of PAR were then estimated by the interpolation methods included in BioCro, as described previously (Humphries & Long 1995) (eqns 9–12). Soil textural classes and depths were assigned from the cited literature (Table 1).

Gas exchange and carbon assimilation

Net leaf CO_2 uptake rate (A) was predicted from the steady-state biochemical model of Farquhar *et al.* (1980) and von Caemmerer & Farquhar (1981), as modified by von Caemmerer (2000), and using the equations of Long (1991) and Bernacchi *et al.* (2001, 2003b) to predict the impacts of climate (temperature, RH, light and CO_2) on ribulose-1:5-bisphosphate (RuBP)-limited and RuBP-saturated photosynthesis (eqns 13–33). The photosynthesis model was coupled with a 'Ball-Berry' model to predict stomatal conductance (Ball *et al.* 1987). Because of the interdependence of photosynthesis, stomatal conductance and leaf–energy balance, an iterative routine was used to simultaneously obtain the best estimate of A , stomatal conductance (g_s) and leaf temperature (T_l) (Humphries & Long 1995) (Supporting Information Table S1, eqns 34–43). At all developmental stages, the canopy was divided into 10 layers of equal leaf area index (LAI). Using hourly recorded PAR, sun angle and leaf

angular distribution, the model estimated the proportion of sunlit and shaded leaves in each of these layers and the average photosynthetically active photon flux density (PFD) of both leaf classes (Humphries & Long 1995; Miguez *et al.* 2009, 2012). From the predicted PFD, temperature and humidity of each leaf class in each layer, carbon, water and heat exchange are predicted and the weighted sum is used to predict total exchange between the whole canopy and the atmosphere for each hour of the day, and each day of the year (Miguez *et al.* 2009) (Supporting Information Table S1, eqns 44–74). To simulate the effect of water stress on stomatal conductance (g_s) when soil water potential falls below a threshold, conductance was reduced as a linear function of available water in the rooting zone (Tezara *et al.* 1999). Parameters used to model these effects of temperature and water stress on stomatal conductance and photosynthesis at the leaf and canopy level for willow are provided in Tables 2 and 3.

Respiration

Growth respiration was assumed to be a constant proportion of net canopy assimilation (Amthor 2000; Miguez *et al.* 2009; Supporting Information Table S1, eqn 75). Maintenance respiration was assumed proportional to the biomass of the leaf, stem and root pools, respectively (Table 2). The temperature dependence of maintenance respiration was estimated using a Q^{10} function. Total respiration was subtracted from canopy assimilation to calculate net primary production on a daily time step (Table 2).

Phenology

The annual cycle of willow growth is described in the model by five phenological phases adapted from Arora & Boer (2005) and Saska & Kuzovkina (2010). These phases are (1) bud burst; (2) the initial spring flush with expansion of leaves; (3) stem elongation of the proleptic branches and the flushing of sylleptic branches; (4) leaf senescence; and (5) leaf fall and dormancy, that is, the period with no leaves. In winter, deciduous trees and shrubs are in a dormant leafless state until temperature is sufficient in the spring to initiate bud burst. Favourable weather in spring triggers trees to enter the initial flush when carbohydrate reserves are mobilized to support the rapid expansion of the leaf primordia present in the overwintering buds. After this spring flush, a slower steady-state growth is attained and assimilated carbon is allocated to the stems and the roots, as well as further leaf production. This is followed by leaf senescence in the fall, where the non-structural leaf organic constituents are mobilized and translocated for storage in the vascular parenchyma of the stem and root. Finally, there is a reversion to the dormant and leafless state until warm weather returns to repeat this five-phase cycle (Arora & Boer 2005). In the model, transition between these phenological stages is controlled by thermal time defined by growing degree days (GDDs), the sum of average daily temperatures with a base temperature of 0°C (Fu *et al.* 2012). A threshold of daily average temperature of

Table 1. Location and management information for the 24 sites used for model calibration and evaluation

Site	Latitude/longitude	Species	Clones	Planting density (m ⁻²)	Growing period	Soil	References
Calibration site							
Uppsala, Sweden	45.5/-89.5	<i>Salix viminalis</i> L.	Two unknown	2	1984–1989	Clay	Lindroth <i>et al.</i> (1994)
Validation sites							
Brumby Farm, Sweden	59.7/16.7	<i>S. viminalis</i> L., <i>S. dasyclados</i> Wimm.	12 clones	2	1990–1994	Clay	Nordh (2004)
Montreal, Canada	45.1/-74.3	<i>S. discolor</i> <i>S. viminalis</i>	Unknown	2	1998–2000	Sandy loam	Labrecque & Teodorescu (2003)
South Sweden	56.9/12.35	<i>S. dasyclados</i> Wimm. <i>S. viminalis</i> L. <i>S. dasyclados</i> × <i>purpurea</i>	075 081 082 206	Not reported	1982–1985	Sand	Christersson (1987)
Pulawy, Poland	51.47/22.07	<i>Salix</i> spp.	Unknown	4	2003–2006	Clay	Borzecka-Walker <i>et al.</i> (2008)
Tully, NY, USA	42.792/-76.125	<i>S. dasyclados</i> <i>S. alba</i> <i>S. alba</i> var. <i>sanguinea</i> <i>S. × rubens</i> <i>S. purpurea</i> <i>S. caprea</i> <i>S. aurita</i> <i>S. schwerinii</i> E. Wolf × <i>viminalis</i> L.	SV1 SA22 SA2 SAM3 SH3 Wild type	1 1	1987–1996	Silt loam	Kopp <i>et al.</i> (2001)
South Bohemia, Czech Republic	49.15/15			58	1994–1995	Clay	Dušek & Květ (2006)
Southwestern Germany	48.733/8.933		Unknown	1	2001–2004	Silty clay	Boehmel <i>et al.</i> (2008)
Abbachhof, Germany	49.08/12.15	<i>S. viminalis</i>	Unknown	2	1983	Sandy clay	Hofmann-Schielle <i>et al.</i> (1999)
Waseca, MN, USA	44.08/-93.51	<i>S. viminalis</i>	Sx-61	2	2004–2006	Clay loam	Randall <i>et al.</i> (2010)
Kwidzyn, Poland	53.67/18.93	<i>S. viminalis</i>	082	4	1996–1999	Clay	Szczukowski <i>et al.</i> (2002)
Balbirnie, UK	56.2419/-3.1812	<i>S. sitchensis</i>	Bebbiana	1	1996–2001	Clay loam	Aylott <i>et al.</i> (2008)
Treifeon, UK	51.9637/-3.2533	<i>S. viminalis</i> × <i>S. schwerinii</i>	Bjorn		1997–2002		
Trumpington, UK	52.1666/0.0926	<i>S. caprea</i> × <i>S. cinerea</i> × <i>S. viminalis</i>	Dasyclados				
Loyton Bampton, UK	51.013/-3.4685	<i>S. burjatica</i>	Delamere				
Llanwrst, UK	53.2341/-4.0139	<i>S. viminalis</i> × <i>S. viminalis</i>	Germany				
Talybont, UK	51.8985/-3.3009	<i>S. viminalis</i> × <i>S. viminalis</i>	Jorr				
Alice Holt, UK	51.1756/-0.8426	<i>S. spæthii</i> <i>S. triandra</i> × <i>S. viminalis</i> <i>S. burjatica</i> × <i>S. viminalis</i> <i>S. viminalis</i> × <i>S. schwerinii</i> <i>S. viminalis</i> × <i>S. viminalis</i> <i>S. viminalis</i> × <i>S. caprea</i>	Jorr Jorun Orm Q83 Spæthii ST2481 Stott10 Stott11 Tora Ulv V789				
Massena, NY	42.8/-76.11	<i>Salix</i> × <i>dasyclados</i>	SV1	1.54	1993–2001	Silt loam	Volk <i>et al.</i> (2011)
Burlington, VT	44.5/-73.21	<i>S. sachalinensis</i>	SX61		2005–2007		
Arlington, WI	43.4/-89.41	<i>S. miyabeana</i>	SX64				
Queenstown, MD	38.6/-76.16						
Waseca, MN	44.1/-93.51						
Boisbriand, QC	45.6/-73.83						
Birch Hills, SK	53.0/-105.4						
Obory, Poland	53.7/18.9	<i>Salix</i> spp.	Unknown	1.8	2004–2007	Clay loam	Stolarski <i>et al.</i> (2013)
Georgenhof, Germany	51.5/9.0	<i>Salix</i> spp.	Unknown	1.5385	1998–2000	Sandy loamy silt	Pacaldo <i>et al.</i> (2013)
Quebec, Canada	45.13/74.13	<i>S. viminalis</i>	5027	2.0	1995–1997	Silt clay	Nissim <i>et al.</i> (2013)
					1998–2001		
					2002–2004		
					2005–2008		

Table 2. Parameters of C_3 model of gas exchange

Parameter description (symbol, unit)	Value	Reference
Maximum Rubisco capacity (V_{\max} , $\mu\text{mol m}^{-2} \text{s}^{-1}$)	100	Wang <i>et al.</i> (2013)
Light-saturated electron transport rate (J_{\max} , $\mu\text{mol m}^{-2} \text{s}^{-1}$)	180	Wang <i>et al.</i> (2013)
Leaf respiration (R_d , $\mu\text{mol m}^{-2} \text{s}^{-1}$)	1.1	Wang <i>et al.</i> (2013)
Stomatal slope factor (m, dimensionless)	5	Wang <i>et al.</i> (2012c)
Stomatal intercept factor (b, dimensionless)	0.08	Wang <i>et al.</i> (2012c)
Atmospheric Pressure (kPa)	103	Long (1991)
Curvature parameter for transition region of A-Q curve (θ , dimensionless)	0.7	Collatz <i>et al.</i> (1992)

Table 3. Parameters governing canopy CO_2 assimilation

Parameter description (symbol, unit)	Value	Reference
Specific leaf area (SLA, ha Mg^{-1})	1.1	Wang <i>et al.</i> (2013)
Extinction coefficient for diffuse light (K_d , dimensionless)	0.37	Casella & Sinoquet (2007)
Height factor or maximum canopy height (m)	10	Miguez <i>et al.</i> (2009)
Coefficient for growth respiration (dimensionless)	0.35	Liu & Bull (2001); Deckmyn <i>et al.</i> (2004)
Q10 factor for leaf maintenance respiration	2.0	Amthor (2000)
Stem maintenance respiration (d^{-1})	0.005	Ryan <i>et al.</i> (1995)
Q10 factor for stem maintenance respiration	1.7	Ryan <i>et al.</i> (1995)
Root maintenance respiration (d^{-1})	0.003	Desrochers <i>et al.</i> (2002)
Q10 factor for root maintenance respiration	1.8	Desrochers <i>et al.</i> (2002)

$\geq 5^\circ\text{C}$ is assumed necessary to allow bud burst in the spring (Bailey & Harrington 2006). Leaf senescence was triggered when accumulated thermal time reached a predefined value, beyond which leaf senescence rate was expressed as a percentage progression per day. Additionally, leaf biomass loss

($Leaf_f$) due to any frost event was expressed as a linear function of ambient temperature (T_a) and current leaf biomass ($Leaf$):

$$Leaf_f = Leaf \times \begin{cases} 0 & T_a > T_1 \\ \frac{(T_a - T_1)}{(T_2 - T_1)} & T_2 \leq T_a \leq T_1 \\ 1 & T_a < T_2 \end{cases}$$

where T_1 represents the temperature threshold for frost damage and T_2 represents the temperature at which total leaf loss occurs. Threshold temperatures of $T_1 = 0$ and $T_2 = -5^\circ\text{C}$ were used (Linkosalo *et al.* 2008).

Partitioning and mobilization of assimilate

Daily net gain in photosynthate by the canopy each day (NPP) is partitioned between stem, root, leaf and the non-structural carbohydrate reserves within the stem and root parenchyma. The proportion allocated to each was controlled by partitioning coefficients, which were calculated from observed partitioning through the growth cycle (Lindroth *et al.* 1994) (eqns 76–90). It was assumed that 5% of stem and root biomass could be remobilized to provide carbohydrate reserves to support the expansion of the initial flush of growth of leaves contained in the overwintering buds (Loescher *et al.* 1990; Landhäusser & Lieffers 2003). This proportion of non-structural carbohydrates in woody stems and roots is consistent with measured quantities in other temperate woody deciduous species (Piper & Fajardo 2011). After completion of expansion, it was assumed that the leaves became the only source of additional carbohydrate to the plant (Table 4).

Planting, coppicing and perennating

The simulation assumed typical SRC willow management: hardwood cuttings of stem segments known as rods were planted and allowed to grow over the first summer and then cut nearly to the ground after leaf senescence to induce multi-stem sprouting from the base in the second year. For a given simulation, the initial stem biomass and planting density at the start of the first growing season was set using literature values where available (Table 1); when not

Table 4. Phenological stages and associated biomass partitioning coefficients. These coefficients were calculated from the data of Lindroth *et al.* (1994). Thermal period, is the interval for each phenological stage in cumulative degree days ($^{\circ}\text{Cd}$) with a base temperature of 0°C ; the first number is the start of the period and the second is the end. Bud burst is assumed to occur once air temperature reaches 5°C . Leaf fall is accelerated once air temperatures of $\leq 0^\circ\text{C}$ occur, as described in *Materials and Methods*

Stage	Thermal period ($^{\circ}\text{Cd}$)	Leaf	Stem	Root	Storage
Bud burst	$T \geq 5^\circ\text{C}$	1	−0.05	0	−0.05
Spring regrowth	0–500	1	0	0	0
Steady-state growth	500–1600	0.15	0.7	0.045	0.105
Leaf fall	1600–3500	0.15	0.7	0.045	0.105
Dormancy/no leaves	3500–	0	0	0	0

reported, planting density was set to 14 350 cuttings/hectare and 0.14 Mg ha^{-1} . This is within the range recommended by Mitchell *et al.* (1999) and a density used in many trials. Coppicing was simulated as the removal of 95% of the stem biomass following leaf senescence (Mitchell *et al.* 1999) (eqn 91).

Model validation

The C_3 photosynthesis sub-model was validated against the leaf gas exchange measurements of Wang *et al.* (2013). There are no published measurements of photosynthesis or production of willow under open-air elevation of $[\text{CO}_2]$ to future conditions. To assess the performance of the sub-model in its response to rising $[\text{CO}_2]$, the output was compared with diurnal photosynthetic measurements made on three poplar species (*Populus* spp.) as a closely related genus. This used the coppiced poplar Free-Air CO_2 Enrichment (POPFACE) study reported by Bernacchi *et al.* (2003a). The parameter values of V_{cmax} and J_{max} were also taken from the same study for simulating photosynthetic performance of three poplar species using values determined in mid-summer, July, but adjusted for temperature at other times of year.

To validate the productivity model, predictions were compared with measurements at 23 study sites in Europe, Canada and the USA (Table 1). These predictions were made using the weather and soil data available for each site. These field trials covered diverse climates, soils and growing conditions across the forested regions of Europe and North America, and included over 30 different genotypes/clones of willow. For plots which were cut back after a single establishment year to initiate a multi-stemmed coppice regrowth, BioCro simulated the establishment year and then a rotation period as reported for the given trials (Table 1; Supporting Information Table S1). Predicted and observed yield was fit by a linear regression model to assess goodness of fit.

Regional predictions of yield in the USA under the current and future atmospheric $[\text{CO}_2]$ with temperature elevation

After multiple site validation of the model for biomass yield, we predicted yields for the contiguous USA. For these simulations, using the STATSGO2 soil database (Soil Survey Staff 2009) and NARR (Mesinger *et al.* 2006) following the procedures outlined in Miguez *et al.* (2012). Simulations were run for 4 year rotations over the contiguous USA for 1979–2010 using hourly weather data for each grid point and at the average atmospheric $[\text{CO}_2]$ for this period of 380 ppm. Yield stability, that is, the variation in yield predicted for any given location resulting from year-to-year variation in weather, was expressed as the coefficient of variation in the harvestable yields across years (standard deviation/mean). To estimate the impact of rising atmospheric $[\text{CO}_2]$, the simulation was repeated at an atmospheric $[\text{CO}_2]$ of 550 ppm. Finally, response to temperature increase was predicted by adding 1 and 2°C uniformly to the historical temperature data from NARR. The effect of elevated $[\text{CO}_2]$ and temperature was

assessed by calculating the percent of yield change due to increase in temperature and $[\text{CO}_2]$ relative to the recorded climate from 1979 to 2010. All simulations assumed no irrigation and that productivity was not limited by nutrient availability or biotic stresses, that is, pathogens, weeds and herbivores.

RESULTS

The predicted leaf photosynthetic rates of leaf CO_2 uptake (A) correlated well with measurements taken in the field for *Salix* × ‘9871-31’ – Sherburne, although slightly overestimating the observed rate (Wang *et al.* 2013) (Fig. 1). The predicted daily variation in A at current and elevated $[\text{CO}_2]$ correlated well with observed A for *Populus alba* [Fig. 2a, $r^2 = 0.90$, RMSE (root mean squared error) = 1.52; $r^2 = 0.81$, RMSE = 4.61], *Populus nigra* (Fig. 2b, $r^2 = 0.80$, RMSE = 2.88; $r^2 = 0.89$, RMSE = 3.64) and *Populus* × *euramericana* (Fig. 2c, $r^2 = 0.83$, RMSE = 3.23; $r^2 = 0.88$, RMSE = 3.97) under fully open-air treatment (Bernacchi *et al.* 2003a).

Simulated dry matter accumulation in stems closely followed observed measurements at the calibration site (Lindroth *et al.* 1994) throughout the growing season in 1986 ($r^2 = 0.72$; RMSE = 3.24) and 1988 ($r^2 = 0.84$, RMSE = 2.38). The model over-predicted dry biomass allocation to leaf, and therefore LAI for the early growing season in both 1986 and 1988. The predicted root biomass was close to that observed in the middle and late growing season in 1988 (Fig. 3). The model effectively captured the trends in biomass dynamics of different plant organs over the year (Fig. 3). The simulation

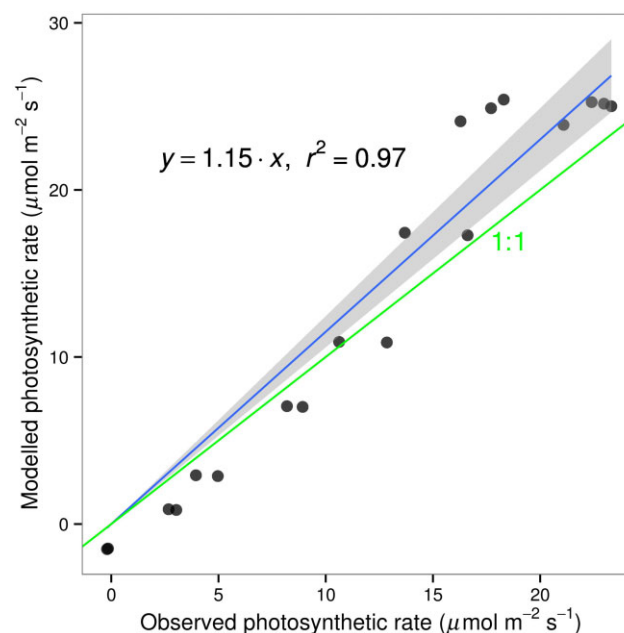


Figure 1. Observed and simulated leaf photosynthetic CO_2 uptake rate (A ; $\mu\text{mol m}^{-2} \text{s}^{-1}$), for different dates and microclimatological conditions. Measurements were taken on *Salix* × ‘9871-31’ – Sherburne on the growing season in 2010 and 2011 in Urbana, Illinois, USA (Wang *et al.* 2013). Shaded area represents 95% confidence intervals of simulated result.

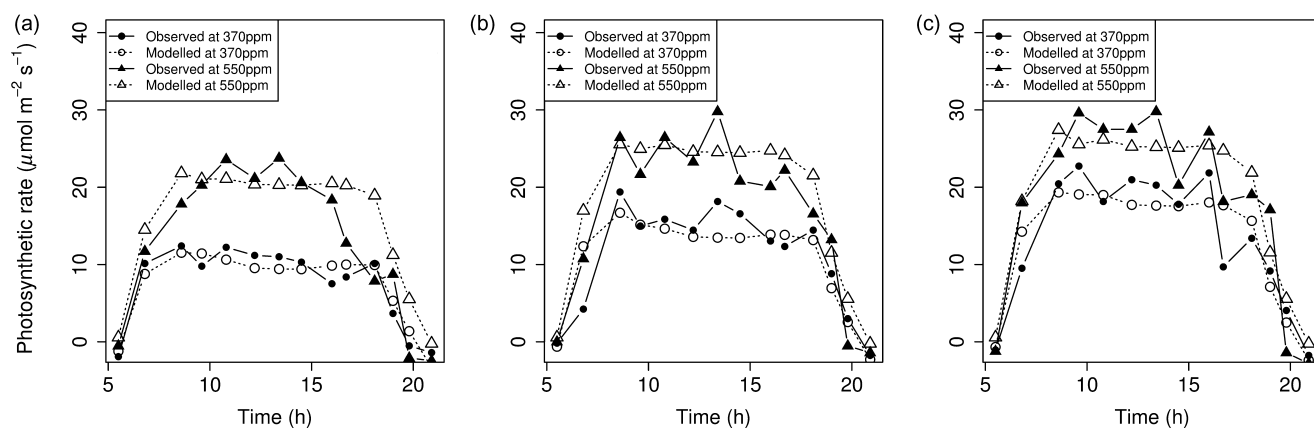


Figure 2. Observed (\blacktriangle \bullet) and predicted (\triangle \circ) rates of diurnal CO_2 uptake (A ; $\mu\text{mol m}^{-2} \text{s}^{-1}$) at ambient (\bullet \circ) and elevated $[\text{CO}_2]$ (\blacktriangle \triangle). Measurements were of *Populus alba* (a), *P. nigra* (b) and *P. x euramericana* (c) on 15 July 2000 at the Free-Air CO_2 Enrichment (FACE) facility near Viterbo, Italy (Bernacchi *et al.* 2003a).

for the two 2 year coppice cycles used in Lindroth *et al.* (1994) at Uppsala, Sweden, is shown in Supporting Information (Fig. S1). Two simulated 4 year coppice cycles following a year of initial growth for Tully, NY, are shown in Supporting Information Fig. S2. Both simulations display similar cycles of leaf production and loss, and accumulation of stem wood, root and storage non-structural carbohydrates; total stem wood is slightly greater and root biomass is almost doubled in the second cycle relative to the first (Supporting Information Figs S1 & S2).

Across the 23 validation sites from 15 studies in Europe and North America (Table 1), there was a close agreement

between simulated and observed standing stem biomass production, as indicated by the alignment with the 1:1 line in Fig. 4 ($r^2 = 0.80$, $\text{RMSE} = 6.3$, $n = 80$). A more detailed comparison with stem biomass measured over two coppice cycles in 6 years across seven sites with contrasting climate conditions also showed good agreement (Fig. 5, $r^2 = 0.67$, $\text{RMSE} = 5.8$, $n = 42$). The predicted mean annual yield for the seven sites was $9.6 \text{ Mg ha}^{-1} \text{ year}^{-1}$, quite close to the observed yield of $8.7 \text{ Mg ha}^{-1} \text{ year}^{-1}$ ($r^2 = 0.88$).

Our regional simulations in the USA predict spatial variability of annual yield of coppice willow across different geographical regions under both current and future atmospheric

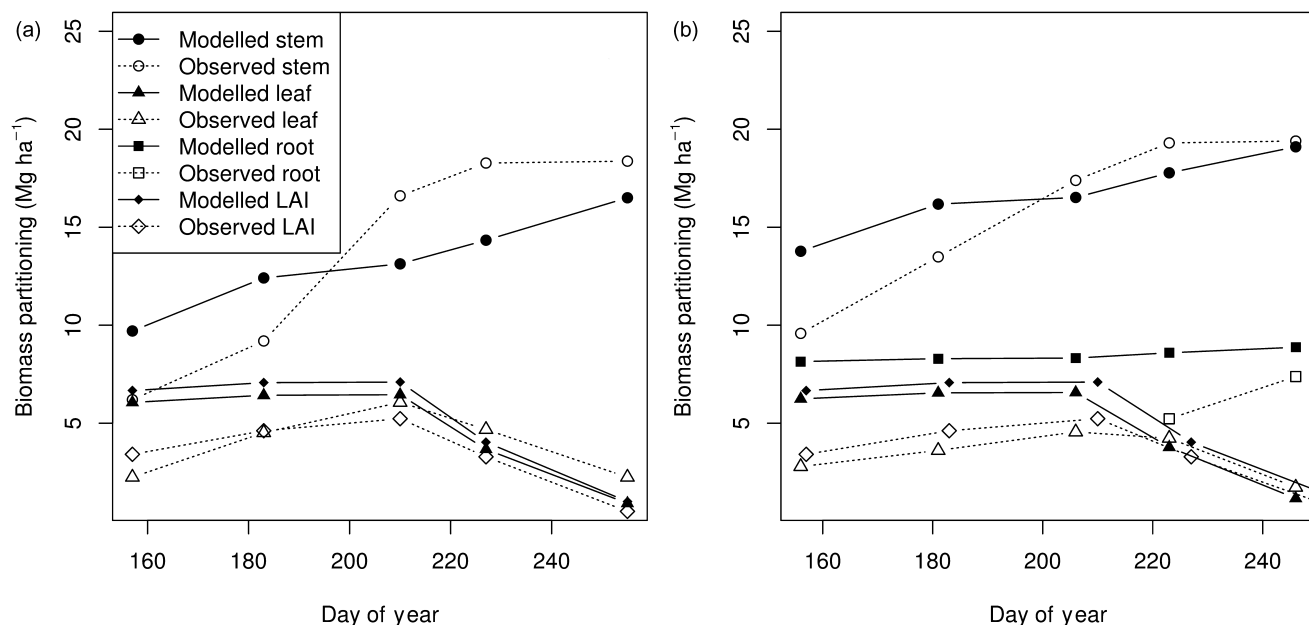


Figure 3. Comparison of BioCro modeled leaf area index (LAI; $\text{m}^2 \text{m}^{-2}$) and standing biomass of stem, leaf and root of willow (Mg ha^{-1}) with measured data throughout the growing season for the second year in the first coppice rotation (a) and the second year in the second coppice rotation (b). Measurements were for *Salix viminalis* L. during the 1986 and 1988 growing seasons in Uppsala, Sweden (Lindroth *et al.* 1994).

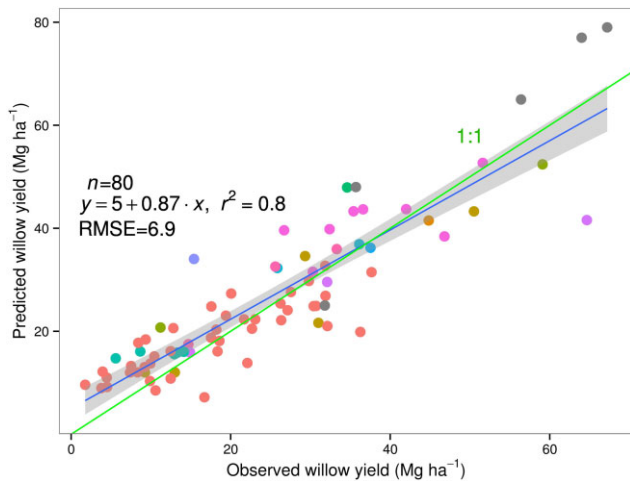


Figure 4. Evaluation of model performance in predicting standing aboveground biomass (Mg ha^{-1}), over varied coppice durations, against independent data collected from multiple sites in Europe and North America (site details in Table 1). Shaded area represents the 95% confidence intervals of the simulated result.

$[\text{CO}_2]$ and temperature conditions (Fig. 6). The highest predicted yields were around $18 \text{ Mg ha}^{-1} \text{ year}^{-1}$; these occurred in the Eastern USA, the upper Midwest, and New England under current climate conditions (Fig. 6a). In contrast, willow is not predicted to produce viable yields in the arid regions of the Western USA; we define viable yield as $\geq 5 \text{ Mg ha}^{-1} \text{ year}^{-1}$ averaged over a 4 year rotation.

The effect of elevated $[\text{CO}_2]$ on the SRC willow yield varied geographically and depended on the magnitude of concurrent temperature increase; with few exceptions (notably the Pacific Northwest, NW), the effect of $[\text{CO}_2]$ declined with increasing temperature (Figs 6 & 7). Elevated $[\text{CO}_2]$ increased coppice willow yield up to 26% at current temperatures (Fig. 7a) and 20% when daily average temperature was increased by 1°C (Fig. 7b). The positive effect of $[\text{CO}_2]$ in isolation from temperature change expanded the range of viable willow yields southward (Fig. 6). However, this positive effect of $[\text{CO}_2]$ on yield was offset by the negative effects of increasing temperature (Fig. 6e,f). Increase in temperature of 2°C decreased SRC willow yield by up to 17% relative to ambient $[\text{CO}_2]$ and temperature depending

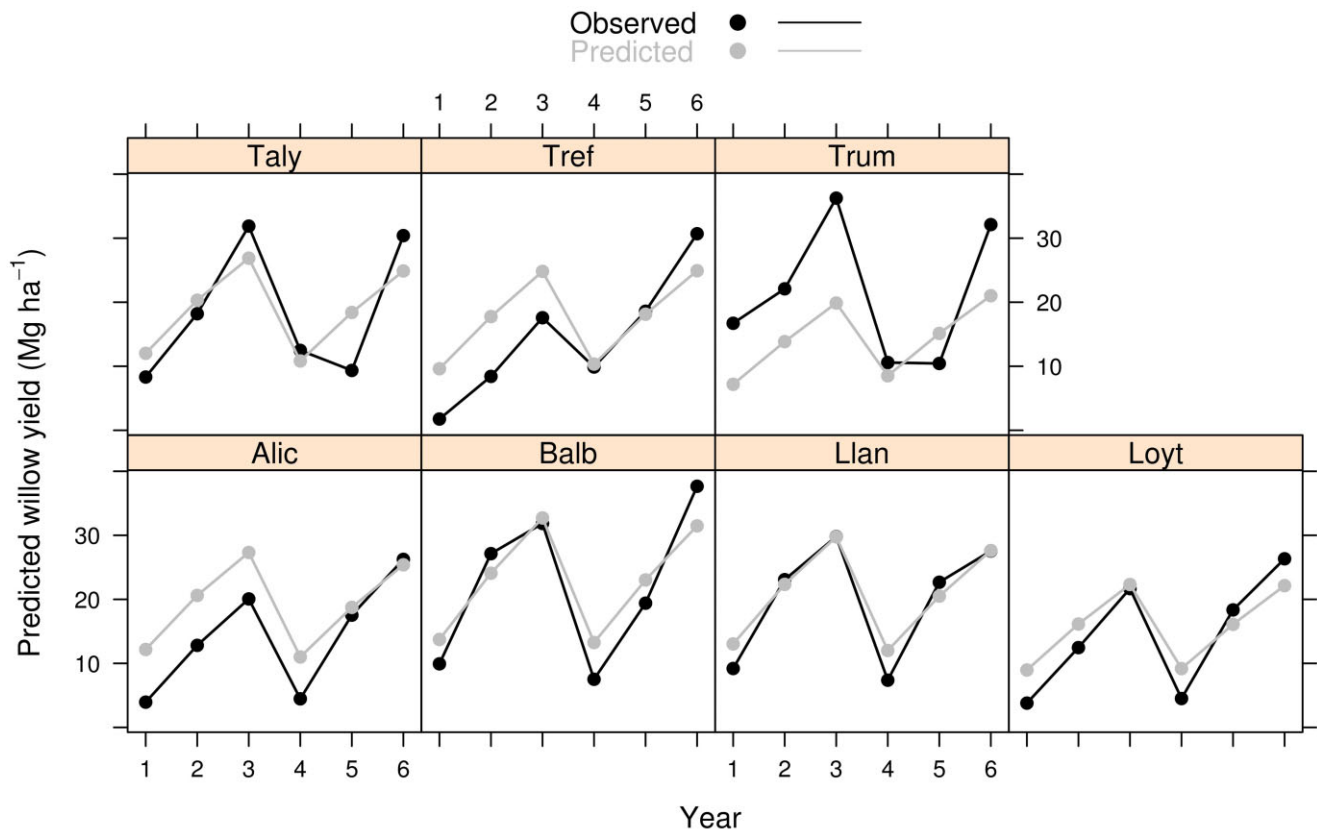


Figure 5. Comparison of BioCro predicted standing stem biomass of willow with the observed standing stem biomass (Mg ha^{-1}) measured from the seven SRC trial sites in the UK from 1996 to 2002. Modeled (●) and measured (○) yields for sites Talybont (Taly), Trefeinon (Tref), Trumpington (Trum), Alice Holt (Alic), Balbirnie (Balb), Llanwrst (Llan) and Loyton Bampton (Loyt) over two 3 year rotations. See Table 1 for site description.

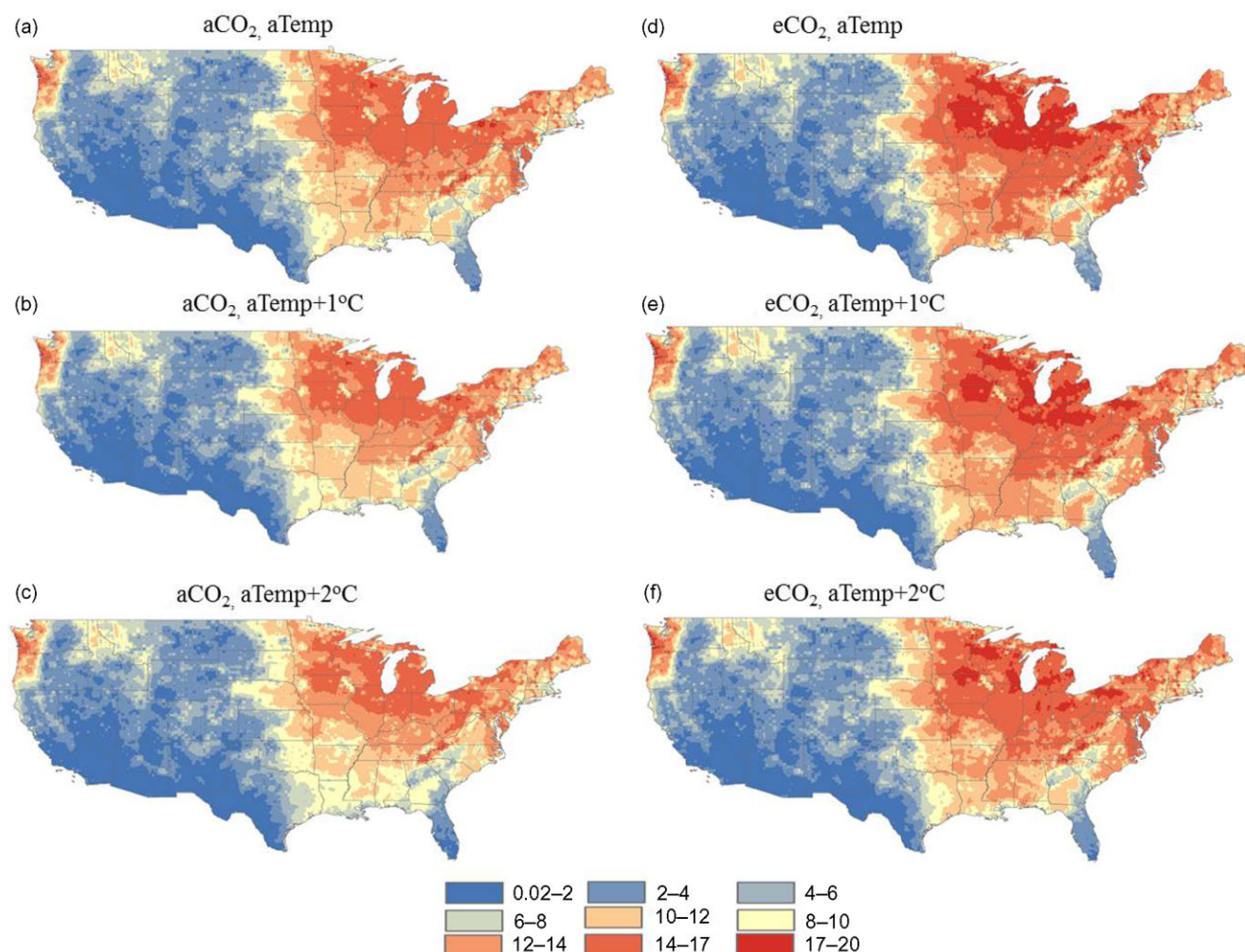


Figure 6. Predicted annualized willow yield ($\text{Mg ha}^{-1} \text{ year}^{-1}$) over a 4 year coppice cycle under current and future elevated $[\text{CO}_2]$ in the USA at different climate scenarios. (a) $[\text{CO}_2] = 380 \text{ ppm}$, temperature = current temperature; (b) $[\text{CO}_2] = 380 \text{ ppm}$, temperature = current daily average temperature + 1°C ; (c) $[\text{CO}_2] = 380 \text{ ppm}$, temperature = current daily average temperature + 2°C ; (d) $[\text{CO}_2] = 550 \text{ ppm}$, temperature = current temperature; (e) $[\text{CO}_2] = 550 \text{ ppm}$, temperature = current daily average temperature + 1°C ; (f) $[\text{CO}_2] = 550 \text{ ppm}$, temperature = current daily average temperature + 2°C (see Supporting Information Fig. S3 for predictions of yield stability calculated from the same model runs).

on location, with the greatest impacts occurring in areas that already produced marginal yields under ambient conditions (Fig. 6c).

Predicted yield stability (indicated by the coefficient of variance, CV) due to year-to-year variability of weather (1979–2010) was correlated to yield, that is, stability was greatest where yield was highest (Supporting Information Fig. S2). Coppice willow yield exceeded switchgrass (Fig. 8a) and Miscanthus (Fig. 8b) in the upper Midwest, Northeast (NE) and Coastal Pacific NW regions.

DISCUSSION

This is the first use of the BioCro modeling framework to simulate the production of either a woody crop or a C₃ crop. After calibration with the detailed physiological, partitioning and production data for a single site, BioCro successfully

predicted yields at 23 other sites from 15 independent studies across a range of soils and climates, providing a successful validation considering that we did not have data to account for the different species and genotypes grown at different sites. The validated model was then used to generate a spatial biomass yield map for SRC willow production in the USA at current and projected future $[\text{CO}_2]$ and temperature conditions. Although there are few studies conducted within the continental USA that could validate this map, the model output appears to track expectation with the best yields in the wetter and cooler areas of the 48 states, including the NE, north central and coastal Pacific NW areas. This study had three specific objectives, which will now be considered in turn.

Objective 1

Develop and parameterize BioCro for willow including the addition or modification of subroutines for coppicing,

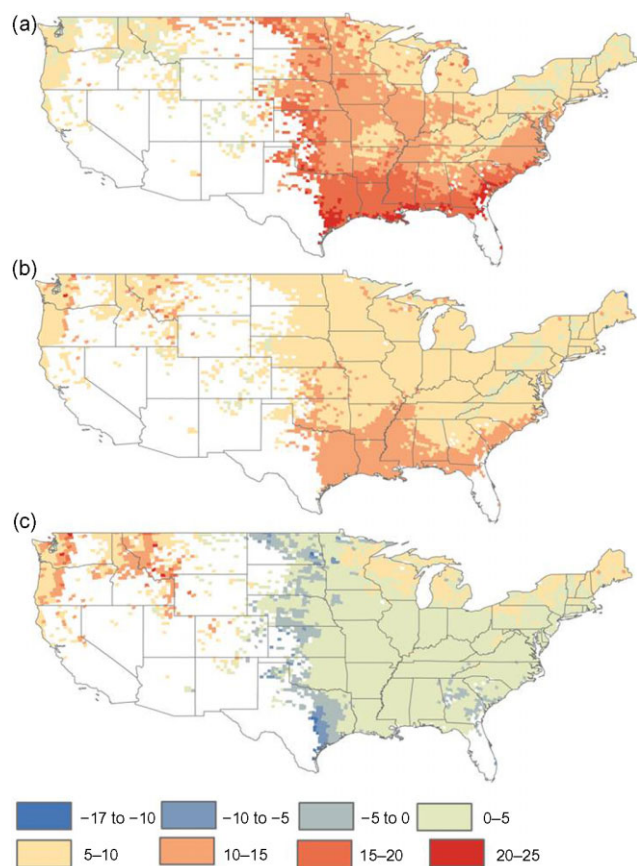


Figure 7. Percentage change in coppice willow yield under elevated $[\text{CO}_2]$ and temperature increase scenarios, compared with coppice willow yield under ambient conditions. (a) Temperature = current daily average temperature; (b) Temperature = current daily average temperature + 1 °C; (c) Temperature = current daily average temperature + 2 °C. Elevated $[\text{CO}_2]$ = 550 ppm. Willow yields lower than 5 $\text{Mg ha}^{-1} \text{ year}^{-1}$ were assumed not to be viable and were excluded from the maps.

woody perennation, C_3 leaf photosynthesis, canopy CO_2 assimilation, allocation, phenology and growth.

We updated the photosynthetic module from WIMOVAC (Long 1991; Humphries & Long 1995) with the temperature response functions of Bernacchi *et al.* (2001, 2003b) and the modifications of von Caemmerer (2000). Willow leaf CO_2 uptake (A) using this approach correlated well with observed data, giving only a slight overestimation (Fig. 1). Poplar and willow growing in similar conditions responded similarly to elevated $[\text{CO}_2]$ (Silvola & Ahlholm 1992; Wang *et al.* 2012b). Because neither of these references reported detailed photosynthetic measurements and associated climate information, we made use of measurements taken on *Populus* spp. in FACE to validate the photosynthetic responses to CO_2 for willow (Bernacchi *et al.* 2003a). The photosynthetic module in BioCro predicted daily variation in A for three *Populus* spp. at ambient and elevated $[\text{CO}_2]$ very effectively, when variation in temperature, RH and photon flux were included (Fig. 2). Although willow grown under elevated $[\text{CO}_2]$ would

have provided a more direct validation of canopy assimilation, there has been no experiment that has examined a willow coppice cycle under open-air elevation of $[\text{CO}_2]$. While a different genus, genomic analysis has now shown large-scale synteny between the two genomes, indicating recent evolutionary divergence (Hanley *et al.* 2007). Further, the averages of the key parameters of the leaf photosynthesis model, J_{max} and V_{cmax} , reported for the poplar species in the POPFACE experiment (Bernacchi *et al.* 2003a) were very similar to the values that we have previously reported for willow (Wang *et al.* 2013).

Allocation of assimilated carbon to different plant organs in BioCro changes dynamically with phenological stage, unlike other models that assume a fixed allocation coefficient to leaf, stem and roots, such as IBIS (Foley *et al.* 1996), ED2 (Medvigy *et al.* 2009; Wang *et al.* 2013), or deduced from allometric relationships or empirical correlation as in BIOME-3 (Haxeltine & Prentice 1996). This is particularly important in a crop production context, since harvest would typically be in the winter and thus would need to realistically represent remobilization of reserves to the wood. This, in turn, will affect prediction of harvested yields and the extent to which stored pools can support regrowth the next spring, as well as the response of the crop to inter-annual variation in climate. Although calibration data for biomass partitioning were only available for a single site and species, *Salix viminalis*, this dynamic partitioning approach effectively simulated stem and root biomass allocation patterns in willow that were consistent with observations throughout the growing season (Fig. 3; Lindroth *et al.* 1994). This was despite the fact that partitioning is influenced by genotypes and environment (Weiner 2004). Recalibration for different genotypes, soils and climates would clearly improve the predictive skill of the model. The leaf phenology scheme in BioCro is a temperature-dependent approach based on thermal time and a threshold temperature to initiate spring bud burst (Sitch *et al.* 2003). This approach effectively predicted bud burst (Supporting Information Figs S1 & S2). LAI was overestimated by the model in the first half of the growing season. Productivity is non-linearly related to LAI, in that increments result in proportionally smaller increments in net canopy carbon gain up to the optimum LAI (Drewry *et al.* 2014). This may explain why, despite overestimation of LAI, there is still a close correspondence of modeled and observed productivity (Fig. 3). This raises the question of why might plants produce more LAI beyond what is required for maximum growth rate. Additional leaves provide insurance against losses to herbivores and diseases, while creating dense shade that inhibits the growth of competitors (Zhu *et al.* 2010; Drewry *et al.* 2014). Indeed, the modeled fraction of aboveground biomass in leaves is similar to other observations for willow (Rytter 2001; Fig. 3). Although photosynthesis declines into the autumn, stem biomass continues to increase as leaf non-structural components are mobilized in senescence and re-absorbed into the stem (Fig. 3).

Coppicing stimulates shoot growth and may avoid the year-on-year decline in annual productivity that occurs as trees and shrubs age. Yields are expected to be greater in the

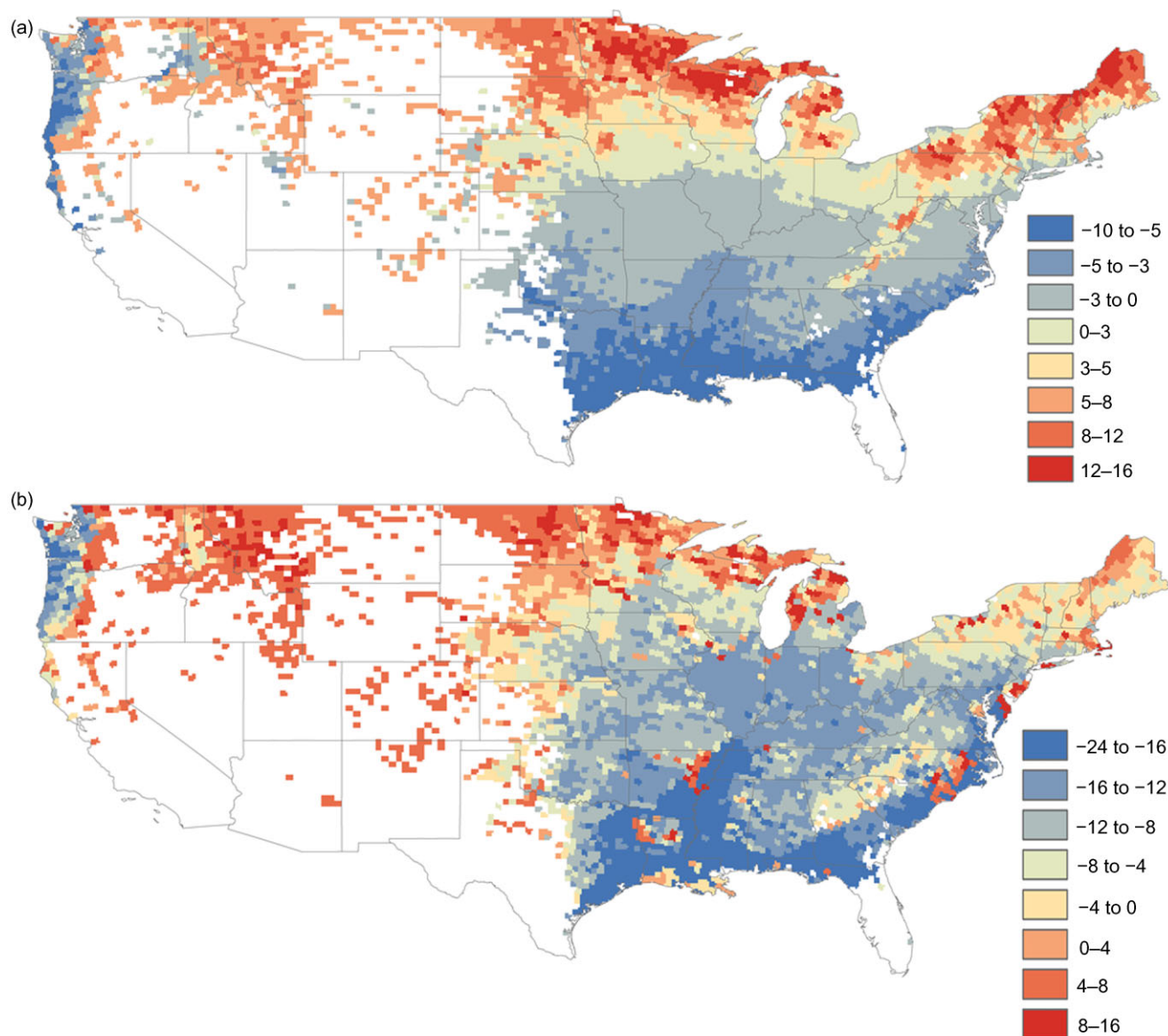


Figure 8. Differences in biomass productivity ($\text{Mg ha}^{-1} \text{ year}^{-1}$) predicted for coppice willow versus switchgrass (a) and *Miscanthus* (b) for the USA. Negative values indicate higher yields for switchgrass and *Miscanthus* production and positive values favour coppice willow. Areas in which willow would yield less than $5 \text{ Mg ha}^{-1} \text{ year}^{-1}$ were excluded from the comparison. Results of switchgrass and *Miscanthus* were those determined with BioCro by Miguez *et al.* (2012).

second harvest rotation compared with the first. This may be attributed to an increase in root biomass and its capacity to store non-structural carbohydrates over the winter that support spring regrowth (Danfors *et al.* 1998). However, among the seven validation sites in the UK, only two exhibited greater yield during the second rotation compared with the first (Fig. 5). At the level of the model, this could be simulated by assuming that the amount of stored non-structural carbohydrate scales with the increase in root system mass obtained by the second cycle (Supporting Information Fig. S2). This would allow greater and more vigorous resprouting following coppicing.

Objective 2

Validate model performance to observations from field trials across diverse locations in the Europe and North America.

Predicted yields were consistent with observed yields at validation sites across Europe and North America, and across a wide range of climates and soils, despite genetic variation between the clones used at the different sites (Figs 4 & 5). From this, we conclude that the model was able to account for the variability in environmental and soil conditions. As calibration was for different clones and species, and the

validation for an even larger range of germplasm, a correlation coefficient (r^2) of 0.8 is unlikely to be improved without genotype-specific parameterization, calibration and validation data. However, it should be appreciated that the predictions are for an average of the historical data, and that new improved cultivars, while showing the same patterns of yield variation, would likely achieve higher yields than shown here. Across seven site trials in the UK (Aylott *et al.* 2008), BioCro overestimated biomass in the first 2 years of the first coppice cycle at two sites and underestimated biomass at a third site. However, biomass predicted by BioCro at the end of the 7 years was within $\pm 10\%$ of the observed biomass at all but one site (Fig. 5). In general, the agreement between modeled and observed data suggests BioCro is a robust model that may be used to predict SRC willow yield in a range of climates and soil conditions. Clearly, it can become more precise as parameterization data become available for specific clones.

Objective 3

To upscale the model to provide high-resolution regional predictions for the USA in current and future $[\text{CO}_2]$ and temperature conditions.

The regional simulations show clear spatial variability of willow yield across the continental USA. As expected, water availability influences predicted yield of willow, the highest yields being achieved in the eastern and upper Midwest, the NE and coastal Pacific NW (Fig. 6) (Davis *et al.* 2012; Wang *et al.* 2013). In most of the West- and South-central semi-arid plains, as well as the warm and cool semi-desert regions of the western interior, willow could not achieve viable yields, which we defined as $\geq 5 \text{ Mg ha}^{-1} \text{ year}^{-1}$ averaged over a 4 year rotation cycle. Despite high rainfall, predicted willow yields were also poor or not viable in the Southeastern USA. In the model, the lower predicted yields in the southeast result from both an accelerated phenology caused by more rapid accumulation of GDDs and greater water vapour pressure deficits that lower water use efficiency. Although these predictions of poor yield in warmer climates are consistent with the observed range over which SRC willow has been successfully established, the precise mechanism that limits the southern extent of willow is uncertain.

We predict that yields of $\geq 14 \text{ Mg ha}^{-1} \text{ year}^{-1}$ are possible over more than 50 Mha in the USA. Much of this area is north and east of the major food crop production areas (Fig. 6). The more productive regions were associated with more stable yields (Supporting Information Fig. S3). Although yields of *Miscanthus* and switchgrass are higher than willow at many locations, coppice willow has greater yield stability at most locations when compared with predictions made with BioCro for these other crops (Miguez *et al.* 2012) owing to the longer harvest cycle, which effectively integrates growth over multiple years.

We predicted an average 26% increase in yields when $[\text{CO}_2]$ is elevated to 550 ppm under the temperatures of the past 30 years (Fig. 7a). This yield enhancement is very close to the 28% average increase in yield reported for trees in a meta-analysis of the FACE experiments with elevation of $[\text{CO}_2]$ to approximately 550 ppm $[\text{CO}_2]$ (Ainsworth & Long

2005). Of particular relevance, the model output was in remarkably close agreement with FACE experiments where 6-year-old SRC poplar achieved a 29% increase in yield at 550 ppm $[\text{CO}_2]$ (Liberloo *et al.* 2006) and aspen volume growth increased 28% by elevated $[\text{CO}_2]$ of 560 ppm (Isebrands *et al.* 1996).

BioCro predicts that warming alone, with ambient $[\text{CO}_2]$, would reduce willow yield (Fig. 6a versus Fig. 6b,c). There are many mechanisms whereby warming alone could decrease crop yield. Within the model, supraoptimal temperatures lower yield by accelerating plant development and shortening phenological stages (Lobell & Gourdji 2012). Elevated temperature in the warmer months can decrease photosynthesis (Wang *et al.* 2012b,c), increase the rate of dark respiration (Ow *et al.* 2008), and increase leaf-to-air water vapour pressure deficit, thereby increasing transpiration and decreasing water use efficiency (Ort & Long 2014). These effects were partly counteracted by simultaneous elevation of $[\text{CO}_2]$ which increased photosynthesis and increased the temperature optimum of photosynthesis (Long 1991). In combination with decreased stomatal conductance, this also acted to increase water use efficiency, allowing production at warmer and drier locations (Fig. 6b,c versus Fig. 6e,f).

Higher proportional responses to elevated $[\text{CO}_2]$ in the temperate region of the Pacific NW were observed in combination with elevated temperature (Figs 6 & 7). This is consistent with findings that elevated $[\text{CO}_2]$ and temperature have a synergistic effect in boosting C_3 photosynthesis when current temperatures are suboptimal (Ainsworth & Rogers 2007). In agreement with the expectation that drought stress is ameliorated due to increases in water use efficiency at elevated $[\text{CO}_2]$ (Long *et al.* 2004; Ainsworth & Long 2005), BioCro predicted a stronger effect of $[\text{CO}_2]$ in the more arid western regions (Figs 6 & 7). The combination of elevated CO_2 and elevated temperatures was shown to increase plant biomass, but the effect may have a threshold of a 5°C increase for dominant species in northern forests (Stinziano & Way 2014). Indeed, the effect of elevated $[\text{CO}_2]$ in these simulations depended on the level of temperature increase, with greater yield stimulation under 1°C than under 2°C temperature increase (Fig. 6e versus Fig. 6f). Together, these results suggest that the extent to which rising $[\text{CO}_2]$ corresponds to rising average temperature will determine whether the most suitable areas for coppice willow growth will shift towards warmer or cooler regions.

Under current climate, coppice willow productivity is expected to exceed that of the highly productive C_4 grasses switchgrass and *Miscanthus* (Miguez *et al.* 2012) in New England, the upper Midwest and Pacific NW regions (Fig. 8). Under future climates, coppice willow may outperform these C_4 grasses over a wider area due to the stronger response of C_3 photosynthesis to elevated $[\text{CO}_2]$ (de Souza *et al.* 2013). For example, in contrast to the 28% average increase in yield reported for shrubs in FACE experiments where $[\text{CO}_2]$ was elevated to 550 ppm (Ainsworth & Long 2005), de Souza *et al.* (2013) observed no increase in *Miscanthus* biomass over 2 years in a FACE experiment that elevated $[\text{CO}_2]$ to 600 ppm. This difference will be particularly notable if

temperature increases are small relative to increase in atmospheric $[\text{CO}_2]$, for example, a 1 °C temperature increase is expected to occur as $[\text{CO}_2]$ increases to 550 ppm (IPCC 2013). Given that plantations of these perennials could be in place for 30 years, and facilities for utilizing the crop longer, understanding how yields will change under expected increases in $[\text{CO}_2]$ and temperature is important in selecting appropriate feedstock for planting and location of planting.

Although the model was calibrated and performed well at independent validation sites across Europe and North America, we identify key areas for future model development and improvement. (1) The genus *Salix* contains approximately 400 species and more than 200 listed commercial and experimental hybrids; genetic variation exists in almost all traits that impact biomass production, allocation and the consequent effect on soil C sequestration. More species-specific or clone-specific data would support more robust parameterization for targeted willow species or cultivars. (2) Knowledge of biomass partitioning is critical to any growth model, and even for a seemingly well-studied species such as willow, data on below-ground biomass dynamics are very limited. This introduces uncertainty that can only be resolved with detailed sampling of root biomass and root growth sufficient to establish dynamics. (3) Field trials used for model validation were mostly located in Europe and the Eastern USA. More data of coppice willow will be needed to validate the model for the south and west in order to improve confidence in continental-scale projections. (4) For the climate change scenarios, the effects of climatic extremes are not taken into account, such as the impact of extreme temperatures and precipitation, and the interactions of climate change with biotic factors such as pests, diseases and weeds; these were not accounted for in this study. Further investigation will determine if the inclusion of such relevant effects and their interactions in BioCro will improve our ability to accurately predict yield of coppice willow. Even without these effects, the high correlation coefficient obtained in validating the model suggests this is a valuable tool for yield prediction and understanding of the mechanisms underlying variation in yield. The mechanistically rich framework also facilitates relatively easy addition of new trait data, for example, those of a new cultivar to assess where it may be of particular value. Further, it also allows the application of optimization routines to predict traits for selection in breeding to achieve higher yield and yield stability within a given geography.

The large-scale deployment of biomass crops for a cellulosic-based biofuel industry requires careful agronomic considerations of spatially explicit potential biomass production. Regional yield predictions were consistent with the limited recorded yields in Europe and North America. Regional prediction maps can be used to identify suitable areas for expansion of coppice willow to meet energy demand, and also to make direct comparisons with other emerging feedstocks, such as *Miscanthus*, switchgrass and sugarcane, within a single modelling framework. This information is also critical in determining the best locations of biorefineries as well as for assessing and mitigating the risk to

feedstock supply. As a mechanistic model, BioCro has the potential to include functional traits to predict the potential of new genotypes/clones of coppice willow, and to predict traits that could increase yields under both current and future climates, based on biochemical, biophysical and physiological understanding.

Mechanistic models encode our understanding of how a system works, allowing us to evaluate our understanding and extrapolate in geometric and climate space beyond what we can observe; however, models are by their nature approximations (Box & Draper 1987). Although we cannot change the nature or limitations of models, we can make our analyses transparent, reproducible and extensible (Peng 2011; Wolkovich *et al.* 2012). As with previous versions of BioCro, we have written this model in open-source languages R and C to make it freely available, easy to use and under version control to facilitate reuse, updating and modification of the model. In addition, the source code and data used to generate the findings presented here are released under an open-source license in the public GitHub repository (<https://github.com/ebimodeling/biocro>). This will enable readers not only to assess and rerun the model in the current version, but also to extend the analysis, use future versions, watch and contribute to the future development (Ram 2013). BioCro can be improved not only through the continued study of evolving knowledge of willow agronomy, genetics and physiology, but also through the genotype-specific parameterizations, improved mechanistic representation of environmental responses, and extension to other crops.

ACKNOWLEDGMENTS

Funding for this research was provided by the Energy Biosciences Institute. We thank Gail Taylor and Matthew Tallis of Southampton University for their help with data sources and initial advice in adapting BioCro to willow.

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Received 23 October 2013; received in revised form 5 March 2015; accepted for publication 5 March 2015

SUPPORTING INFORMATION

Additional Supporting Information may be found in the online version of this article at the publisher's web-site:

Figure S1. BioCro modeled standing dry mass of stem, leaf, root and storage pool of willow (Mg ha⁻¹) and leaf area index (m² m⁻²). Simulations were conducted for *Salix viminalis* L. following the establishment year in which the main stem had been cut to encourage branching. Depicted are years 2–5, the first two coppice cycles, with harvests (arrowed) at the end of years 3 and 5 at Uppsala, Sweden (Lindroth *et al.* 1994). Measurements were taken in years 2 and 4, as shown in Fig. 3.

Figure S2. Illustrating the coppicing and harvesting schemes used in the regional simulations, with the site in Tully, NY (2004–2012), as an example. As is standard practice, the main stem was cut at the end of year 1 to encourage branching that then harvesting was conducted on a 4 year coppice cycle, that is, at the end of years 5 and 9.

Figure S3. Coefficient of variability in willow yield due to year-to-year weather variation across the 48 states using the climate data of 1979–2010. To predict climate change

impacts, a fixed increase in temperature or/and $[\text{CO}_2]$ was added to the recorded data. (A) $[\text{CO}_2] = 380$ ppm, temperature = current temperature; (B) $[\text{CO}_2] = 380$ ppm, temperature = current daily average temperature + 1 °C; (C) $[\text{CO}_2] = 380$ ppm, temperature = current daily average temperature + 2 °C; (D) $[\text{CO}_2] = 550$ ppm, temperature = current temperature; (E) $[\text{CO}_2] = 550$ ppm, temperature = current

daily average temperature + 1 °C; (F) $[\text{CO}_2] = 550$ ppm, temperature = current daily average temperature + 2 °C. a = temperature or/and $[\text{CO}_2]$ conditions of the period 1979–2010; e = elevated temperature or/and $[\text{CO}_2]$, as indicated.

Table S1. The equations used in BioCro to simulate SRC Willow, parameter definitions and parameter values.