1   Modelling the carbon cycle of *Miscanthus* plantations: existing models and the potential for
2   their improvement
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4   Modelling *Miscanthus* C cycles
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30   Research Review

<u>Abstract</u>

The lignocellulosic perennial grass *Miscanthus* has received considerable attention as a potential bioenergy crop over the last 25 years, but few commercial plantations exist globally. This is partly due to the uncertainty associated with claims that land use change (LUC) to *Miscanthus* will result in both commercially viable yields and net increases in carbon (C) storage. To simulate what the effects may be after LUC to *Miscanthus*, six process-based models have been parameterised for *Miscanthus* and here we review how these models operate. This review provides an overview of the key *Miscanthus* soil organic matter models and then highlights what measurers can do to accelerate model development. Each model (WIMOVAC, BioCro, Agro-IBIS, DAYCENT, DNDC and ECOSSE) is capable of simulating biomass production and soil C dynamics based on specific site characteristics. Understanding the design of these models is important in model selection as well as being important for field researchers to collect the most relevant data to improve model performance. The rapid increase in models parameterised for *Miscanthus* is promising but refinements and improvements are still required to ensure model predictions are reliable and can be applied to spatial scales relevant for policy. Specific improvements, needed to ensure the models are applicable for a range of environmental conditions, come under two categories: 1) increased data generation and 2) development of frameworks and databases to allow simulations of ranging scales. Research into non-food bioenergy crops such as *Miscanthus* is relatively recent and this review highlights that there are still a number of knowledge gaps regarding *Miscanthus* specifically. For example, the low input requirements of *Miscanthus* make it particularly attractive as a bioenergy crop but it is essential that we increase our understanding of the crop's nutrient re-mobilisation and ability to host N-fixing organisms in order to derive the most accurate simulations.

Introduction

Interest in the C4 perennial grass *Miscanthus* as a renewable energy source has grown significantly over the last two decades. *Miscanthus* has great potential for large scale deployment as a bioenergy crop, used either for electricity generation in power stations, or as a future renewable source of bioethanol (Heaton *et al*., 2008; Karp and Richter, 2011). It is native to South and East Asia, but has been shown to often produce high yields without fertiliser input across Europe and North America, and is tolerant to a range of climatic conditions (Clifton-Brown *et al*., 2004; Dohleman and Long, 2009; Strullu *et al*., 2011; Poeplau and Don, 2013). If *Miscanthus* plantations are established for bioenergy purposes, land use change (LUC) is inevitable and the influence that LUC has on soil carbon stocks and greenhouse gas (GHG) emissions is a key component of assessing sustainability within a bioenergy context. Carbon (C) accounting as a site management practice is becoming increasingly important (Borak *et al*., 2013) and consequently models need to become better in representing the full C cycle. Modelling of C dynamics in terrestrial ecosystems will undoubtedly become more comprehensive over time, but we are currently limited, not by our knowledge of the processes governing C transfer, but rather by the availability of reliable field data and high resolution large spatial datasets to test that understanding. This empirical data can be used to either validate the processes that govern a model's simulation, or to verify the model's outputs and predictions. Therefore, a lack of validation data also means a lack of verification data, thereby creating questions about uncertainty quantification of current simulations.

Modelling studies consistently report an increase in soil C stocks after LUC from most different land uses into *Miscanthus* (Don *et al*., 2012; Mishra *et al*., 2012) but empirical

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studies of LUC to *Miscanthus* show mixed results: some show a notable increase in topsoil

soil C stocks each year (Hansen *et al*., 2004) whereas others report no significant increase

(Schneckenberger and Kuzyakov, 2007; Zimmermann *et al*., 2012; Zatta *et al*., 2013) or

various changes including reductions (Poeplau and Don, 2013). Consequently, this

discrepancy needs to be addressed so accurate predictions can be made about the

environmental impacts of the LUC and the C budgets associated with *Miscanthus* plantations.

Such uncertainties have helped contribute to the limited establishment of *Miscanthus* and it is

imperative that before wide-scale deployment is undertaken, model outputs are verified by

robust and wide-ranging field data. These empirical data are also needed to underpin

validation of the mechanistic aspects of models predicting biomass yields and ecosystem C

dynamics, with improved validation leading to reduced uncertainty.

Validating model processes and verifying their outputs is particularly difficult for emerging

non-native crops, like *Miscanthus*, as relevant field data is scarce. Current literature

highlights that a lack of field data has limited 1) effective model parameterisation, 2) the

quantification of model uncertainty, 3) inter-model comparisons and 4) the eventual

application of *Miscanthus* models (Clifton-Brown *et al*., 2007; Miguez *et al*., 2009; Hastings

et al., 2009b; VanLoocke *et al*., 2010; Cuadra *et al*., 2012; Miguez *et al*., 2012; Surendran

Nair *et al*., 2012).

The last decade has seen a rise in the number and sophistication of mechanistic models

capable of simulating C dynamics of *Miscanthus* plantations, but there are still aspects of

these models that can be improved. These include, but are not limited to, the longevity of soil

C stocks and specifically newly sequestered soil C (Dondini *et al*., 2009), C losses and gains

from roots, shoots and leaves individually (Foereid *et al*., 2004; Amougou *et al*., 2011),

106 nutrient remobilisation and associated N-fixation (Eckert *et al*., 2001; Cadoux *et al*., 2012;

107 Keymer and Kent, 2013) and the increased uncertainty when scaling up simulations to larger

108 spatial scales (Pogson, 2011). A number of applicable models have recently been reviewed

109 by Surendran Nair *et al*. (2012), providing detailed model descriptions of how the models

110 simulate biomass production and soil water, nutrient and C cycle dynamics for bioenergy

111 crops in general. However, in this review, we focus the discussion only on models that have

112 been parameterised and validated for *Miscanthus* simulations and specifically what

113 measurements are required to improve model performance regarding soil C aspects of the C

114 cycle. In addition to two models (WIMOVAC and Agro-IBIS) also discussed by Surendran

115 Nair *et al*. (2012), we review four other models suitable for *Miscanthus* C studies (BioCro,

116 DayCent, DNDC and ECOSSE). Further, we briefly discuss the current databases available

117 for use with the models described and possible frameworks that may encourage and

118 accelerate model development.

119

120 **Identifying existing models parameterised for *Miscanthus***

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122 A literature search was performed to identify existing C budget models that fulfilled all of

123 five criteria. Models were required to be: 1) mechanistic in design, 2) parameterised and

124 validated for *Miscanthus* plantations, 3) capable of both predicting crop yields and soil C

125 dynamics, 4) published in a peer-reviewed journal or conference proceedings and 5) report

126 outputs validated against field data. Mechanistic models were specifically chosen to allow

127 greater flexibility when simulating the impacts of future climatic scenarios and changing

128 environmental conditions. Similarly, mechanistic models are more transferable to the larger

129 geo-spatial scales that policy decisions are often created for. Consequently, mechanistic

130 models can play an important role in deciding whether *Miscanthus* is an appropriate crop for

131 geographically distinct regions (i.e. their climate and soil properties). Additionally, the ability

132 for the models to simulate both yields and soil C dynamics was required because assuring the

133 commercial viability of a *Miscanthus* plantation, and assessing its impact on net C emissions,

134 are essential parts of a landowner choosing to establish *Miscanthus* over a more conventional

135 crop.

136

137 We identified five crop growth models parameterised for *Miscanthus*: WIMOVAC (Miguez

138 *et al*., 2009), BioCro (Miguez *et al*., 2012), Agro-IBIS (VanLoocke *et al*., 2010), DayCent

139 (Davis *et al*., 2010) and DNDC (Gopalakrishnan *et al*., 2012). In addition, the ECOSSE

140 model (Smith *et al*., 2010a) is included as it is currently being adapted to simulate C budgets

141 in a *Miscanthus* plantation (Jones *et al*., 2011). Of these models, WIMOVAC, BioCro and

142 Agro-IBIS were originally created to simulate biomass production but have more recently

143 had soil biochemistry and soil C incorporated in their simulations. Conversely, DayCent,

144 DNDC and ECOSSE were all principally designed to simulate belowground nutrient cycling

145 and have only included more complex plant growth routines recently.

146

147 **Considerations for *Miscanthus* model selection**

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149 There are many factors to consider regarding model selection and here we highlight the key

150 considerations for modelling *Miscanthus* C dynamics. We group these considerations into

151 four categories: 1) model parameters, 2) scale, 3) inputs and 4) verification of model outputs.

152 The models presented vary greatly in their approach to simulate the same ultimate outputs.

153 For example, DayCent uses a continuous phonological development curve to allocate C

154 assimilated into five pools of biomass (Davis *et al*., 2010), whereas Agro-IBIS applies three

155 discrete development stages to calculate crop growth and partitions the C into three pools of

156 biomass (VanLoocke *et al*., 2010). Both approaches are valid but there are advantages and

157 disadvantages to each which are discussed during Section 2 of this review. The general

158 characteristics of each of the six models reviewed here are summarised in Table 1.

159

160 *Model parameters*

161

162 The research objective for a model may be to quantify a set variable but it is possible that the

163 chosen model a) lacks the desired output (i.e. change in C stocks) or b) does not describe the

164 output at the soil depth and/or timescale required (i.e. monthly change to the active soil C

165 fraction/change in C at a certain soil depth increment). Therefore, early consideration of the

166 models' functionality is required to match expectations for use. As an example, WIMOVAC

167 would be unsuitable to evaluate temporal variation between soil CO_2 emissions and soil C

168 content as the model calculates C losses by assuming a fixed fraction is lost and, relative to

169 total C accumulation, C losses will always be the same.

170

171 It is worth noting that the model parameters that determine many aspects of C transfer within

172 the system (e.g. C assimilation, growth rates of the crop and SOM turnover rates) may change

173 depending on the genetic variation of the *Miscanthus* species. The models discussed here

174 have been parameterised and verified for *Miscanthus giganteus* and/or *Miscanthus sinesis*,

175 but a number of genetic variants are being trialled in the UK to improve biomass production

176 in less-than-optimal climatic conditions (Clifton-Brown *et al*., 2008; Robson *et al*., 2011).

177 Studies indicate that it is possible that different genetic variants may respond differently to

178 abiotic stresses (Borzęcka-Walker *et al*., 2008). Similarly, it is plausible that litter quantity

179 and quality will vary, influencing C inputs to the soil. Consequently, to accurately simulate

180 crop growth and associated ecosystem C dynamics from these new variants, the existing

181 models may need to be re-parameterised when sufficient field data is available.

182

183 *Inputs*

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185 As well as considering the desired outputs for a model it is also important to ensure that the

186 required data inputs to the model are readily available. All of the six models reviewed require

187 inputs of site soil properties (Table 2) meaning if this data is unavailable for the desired

188 resolution (see section *1.2.3. Scale*) the model outputs may not be reliable. Similarly, five of

189 the six models are able to interpolate daily inputs of known site characteristics when

190 additional data are unavailable, whilst DayCent can only interpolate monthly inputs.

191 Consequently, certain models will be more appropriate than others depending on the research

192 question. The input data available to a modeller is an important consideration when choosing

193 a model just as is the importance of ensuring any new data collection meets the demands of

194 the chosen model. Therefore, knowing the input requirements of relevant models is an

195 essential part of selecting the most appropriate model. Table 2 lists both the essential and

196 optional inputs of each model, therefore simplifying the model comparison when choosing.

197 For a model to operate to the highest attainable degree of accuracy, all required and optional

198 inputs are suggested.

199

200 *Scale*

201

202 If a model has been created to operate at a certain spatial scale, the assumptions made, and

203 conclusions that can be drawn, may not be valid at different spatial scales. Similarly, if high

204 resolution temporal outputs are required, some models are able to interpolate this data while

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205 others are not. All of the models discussed in this review operate at high temporal resolutions

206 (daily time step or more frequently) but there is a greater variation among them with regards

207 to the geo-spatial scales they were originally designed to operate at (see Table 1). Many of

208 the models require site-specific conditions as inputs to drive the simulations, meaning that

209 using information from a single site to represent a larger area will likely be an oversimplified

210 approximation, resulting in unreliable projections. However, recent studies that attempt to

211 upscale the models to large geo-spatial regions indicate reliable simulations can be driven

212 with current databases. For example, MISCANFOR (Hastings *et al*., 2009a) - a mechanistic

213 model designed to simulate *Miscanthus* biomass production - has been successfully used to

214 simulate *Miscanthus* growth over 25 km grids using a number of different datasets for

215 meteorological inputs and soil characteristics (Hastings *et al*., 2009b; Pogson, 2011; Pogson

216 *et al*., 2012; Pogson *et al.*, 2013). The model outputs were then related to geographic

217 information system (GIS) maps at European and global scales with good agreement against

218 empirical field data.

219

220 The MISCANFOR model uses many of the same inputs of soil and meteorological data that

221 the six models reviewed in this paper do, therefore indicating that each may cope with

222 upscaling with similarly accurate outputs using the same datasets. That said, at present there

223 is no robust dataset for soil C stocks at high spatial resolution and without this dataset models

224 can only provide part of the ecosystem C budget. It is worth noting that generally, the fewer

225 inputs required to drive the model, the easier the model will be to scale up to represent larger

226 areas due to the limited number of databases available, but the less mechanistic the model,

227 the less transferable its simulations are over large geo-spatial regions. Therefore, when

228 applying a model to large spatial scales, some trade off will always occur between the

229 datasets available and the inputs required by a model to achieve the highest accuracy

230 simulations. Most of the six models reviewed here have only been validated extensively at

231 site scales. However Agro-IBIS is a dedicated dynamic global vegetation model (DGVM),

232 and therefore is likely to be the most straightforward if the simulation of LUC, to and from

233 other plant functional types, is required over ecosystem scales.

234

235 *Verification of model outputs*

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237 At the field or plot scale, verifying a model's reliability requires independent experimental

238 verification data from the same location (Smith & Smith, 2007). However, since one of the

239 main purposes of modelling is to upscale beyond measurement capacities (space and time),

240 model verification through field data is often not possible. Therefore it is important to ensure

241 that model outputs have been verified within a range of conditions to reflect the sites and land

242 uses under consideration. Although the models reported in this review have been validated

243 for various site conditions, there may be additional variables not included, or those described

244 ineffectively. For example, Davis *et al*. (2010) found that parameters controlling the DayCent

245 model's N-cycling simulation were insufficient for simulating *Miscanthus* growth at sites in

246 Illinois, USA. Further experimentation concluded that the plant, or microbial symbioses,

247 were fixing N which was, in turn, influencing yields. Consequently the DayCent model was

248 calibrated to describe N-fixation differently, accounting for the experiment's findings.

249 Overall, since *Miscanthus* propagation is relatively recent, there is likely to still be much we

250 do not know, particularly with regards to the retranslocation of nutrients after the crop's

251 growth phase (Beale and Long, 1997; Beuch *et al*., 2000) and potential N-fixation from the

252 crop's association with N-fixing organisms (Keymar and Kent, 2013). This emphasises the

253 importance of researchers collecting targeted field data that can be used to accelerate model

254 development and validation (Zhang *et al*., 2010; Surendran Nair *et al*., 2012).

Models parameterised for *Miscanthus*

The six models identified share a number of similar internal components and represent many of the same ecosystem processes, albeit in different ways or with different levels of complexity (Table 1). For example, all of the models simulate plant growth, but only DayCent calculates Net Primary Productivity (NPP). The other models estimate C assimilation based on solar interception and *Miscanthus*-specific photosynthetic efficiency. Although the outputs from the models are similar, there are differences in how the C dynamics are simulated and allocated to plant biomass or soil C pools. In this section we give an overview of the six *Miscanthus* models and suggest the field data most relevant for improving model performance. Much of the discussion of model improvement is focussed on validating predictions of changes to soil C, nutrient translocation and N-fixation ─ the aspects of *Miscanthus* modelling where increased empirical data and improved understanding will have the greatest benefit on future simulations.

Selected model descriptions

WIMOVAC and BioCro

First created as a generic crop growth model (Humphries and Long, 1995), WIMOVAC was parameterised for a *Miscanthus* plantation in England, UK and shown to realistically simulate biomass production at a number of discrete sites with varying climatic conditions across Europe (Miguez *et al*., 2009). More recently, a new version of WIMOVAC named BioCro has been developed; this is written in the programming language *C*, with an interface to work with it using the statistical package *R*. BioCro has since been used to simulate *Miscanthus*

280 biomass production across the contiguous United States (Miguez *et al*., 2012). Both versions

281 represent biophysicochemical processes in detail and operate at an hourly time step, with

282 some processes and state variables updated sub-hourly (e.g. C assimilation) (Humphries and

283 Long, 1995). Parameterised for *Miscanthus*, the models follow a phenological growth routine

284 comprising six development stages in accordance with the typical growth phases of grasses

285 reported by Cao and Moss (1997): emergence, juvenile, induction, post-induction, flowering

286 and post-flowering (Miguez *et al*., 2009). Progression through these stages is controlled by

287 thermal time, or degree days (DD) and the growing season is defined as being from the last

288 frost of the spring to the first frost of the autumn in accordance with Price *et al*. (2004).

289

290 Both models are calibrated for C4 photosynthesis and use the biochemical approach of

291 Collatz *et al*. (1992) for simulating the photosynthetic potential of the crop. Here, they

292 calculate gross photosynthesis as a function of leaf temperature, intercellular CO_2 partial

293 pressure, and incident solar radiation. WIMOVAC and BioCro define the light extinction

294 coefficient (k) using the sunlit and shade classes defined by Norman (1980) but applying an

295 additional parameter to describe the ellipsoid arrangement of leaves (Miguez *et al*., 2009;

296 Miguez *et al*., 2012). Further, the models divide the canopy into ten layers and compute the

297 radiative conditions for each. The canopy function in BioCro can also be used to obtain

298 information about assimilation, transpiration and conductance at different canopy levels.

299 Biomass production is then simulated and allocated to four pools (leaf, stem, rhizome and

300 root) according to fixed partitioning parameters specific to the phenological stage. Although

301 WIMOVAC and BioCro are similar in many ways, biomass partitioning coefficients are

302 handled differently, with BioCro capable of applying negative coefficients for all biomass

303 pools. Additionally, one specific difference concerns the magnitude of C translocation away

304 from the rhizome during the emergence and juvenile stages: WIMOVAC uses coefficients of

305 -0.1 and -0.08, respectively, whereas BioCro uses -0.0008 and -0.0005 for the earliest two

306 stages, respectively. Further, BioCro has been modified to ensure positive and negative

307 allocation coefficients sum to zero. Both models also separate the respiration associated with

308 crop growth from respiration associated with crop maintenance, using a constant related to

309 the plant structure (Miguez *et al*., 2009).

310

311 In addition to C allocation within the crop biomass, C dynamics are also simulated for soil

312 pools. The models separate soil C into active, slow and passive pools according to those of

313 CENTURY (Parton *et al*., 1993). C losses from gaseous emissions and leaching are also

314 accounted for by both models (Humphries and Long, 1995; Miguez *et al*., 2012). The models

315 only account for mineralisation and immobilisation of nitrogen (N) thereby providing

316 necessary information about N availability, but not a full account of the N budget. Similarly,

317 soil water routines and the hydrological sub-model include only variables for the most

318 important processes (Table 1). Since *Miscanthus* biomass production has been shown to be

319 influenced greatly by water availability (Clifton-Brown and Lewandowski, 2000; Heaton *et

320 al*., 2004; Richter *et al*., 2008; Oliver *et al*., 2009), it is worth noting that both WIMOVAC

321 and BioCro use an empirical water stress response function based on that of Boyer (1970) but

322 also accounting for the system's energy balance and present growth phase. This function

323 reduces stomatal conductance through a linear relationship to leaf water potential and soil

324 moisture content, then alters biomass partitioning to roots when the *Miscanthus*-specific

325 average daily plant water potential is below a fixed threshold value (Long *et al*., 1998).

326 However, neither of the models account for stem death during periods of extended water

327 stress (Miguez *et al*., 2009).

328

329   WIMOVAC and BioCro are very detailed mechanistic models, defining biophysiochemical

330   interactions by the underlying processes. This makes both models advantageous in their

331   transferability since the underlying processes do not change over spatial or temporal scales

332   but disadvantageous when noting the substantial amount of data required to initialise the

333   model for a specific site (Miguez *et al*., 2012). As a result, both models rely heavily on data

334   published in only a few studies (e.g. Beale and Long, 1995; Beale *et al*., 1996; Naidu *et al*.,

335   2003). Consequently, to improve WIMOVAC or BioCro the most beneficial data would be

336   that which could verify model outputs under environmental conditions discrete to those

337   already reported. Intra-annual measurements of CO_2 uptake rates and leaf area index (LAI),

338   along with biomass accumulation in the four pools represented by the models would ensure

339   validation of the key parameters influencing C assimilation as well as verification of the

340   model's outputs for biomass production and partitioning. A greater understanding of this

341   partitioning can help us to know when is the right time to harvest aboveground biomass,

342   maximising the landowner's profits for a given year and acknowledging that inter-annual

343   variability can influence *Miscanthus* yields by 10-25% (Price *et al*., 2004; Christian *et al*.,

344   2008). Typically, *Miscanthus* is harvested in early spring as the combustion quality of the

345   biomass is higher and specifically the moisture content of the biomass is lower

346   (Lewandowski and Kicherer, 1997; El Bassam and Huisman, 2001; Lewandowski and Heinz,

347   2003; Lewandowski *et al*., 2003a). Unfortunately, since neither WIMOVAC nor BioCro

348   currently simulate moisture content of the crop biomass, they cannot be used to predict the

349   optimum harvest time with regards to moisture content. However, using a sorption model,

350   such as the modified Oswin model used by Arabhosseini *et al*. (2010), coupled with the air

351   temperature and relative humidity parameters already included within WIMOVAC or

352   BioCro, moisture content for *Miscanthus* could be estimated depending on the environmental

353   conditions of a specific site for a specific year. Unlike the issue of biomass moisture content,

354 quantifying *Miscanthus'* unique properties regarding nutrient retranslocation and N-fixation

355 is not so easily resolved within the models. That said, both models have had multisite

356 validation and been verified against a number of sites across the USA, indicating that the

357 current parameterisation and calibration of the models is at least accurate within the range of

358 environmental conditions present in this region. However, empirical data regarding soil C

359 stocks are still scarce and therefore to date there is no literature citing WIMOVAC or BioCro

360 being used to simulate changes in soil C from sites discrete to those used to parameterise or

361 initialise the models.

362

363 *Agro-IBIS*

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365 Agro-IBIS is a DGVM and unlike the other models in this review, is calibrated to use grid-

366 based simulation techniques to function at large spatial scales. The original model (Foley *et*

367 *al.*, 1996) was designed to apply the same agroecological rationales from models operating at

368 a site scale but draw conclusions about the growth and management of crops at scales often

369 required for policy making (Kucharik, 2003; Kucharik and Byre, 2003). VanLoocke *et al.*

370 (2010) parameterised Agro-IBIS for *Miscanthus* and reported both the default and new values

371 for any altered internal parameters. The model does not employ *Miscanthus*-specific

372 phenological development stages but rather the model retains three stages that have been used

373 successfully to simulate maize biomass production: budburst, senescence and dormancy.

374 Although this is a generalisation of the phenology for the given plant functional type, many

375 aspects of biomass production are similar for maize and *Miscanthus* (Dohleman and Long,

376 2009), and Agro-IBIS adjusts parameters to affect the timing of these events accordingly

377 (VanLoocke *et al.*, 2010).

378

379   The *Miscanthus* version of Agro-IBIS uses the specific leaf area (SLA) approach (Adam *et*

380   *al*., 2011) to estimate total leaf area for the crop, assigning a constant value according to

381   Dohleman and Long (2009). The light extinction coefficient (k) is then estimated according to

382   incident radiation, surface albedo, leaf area and leaf orientation (Kucharik and Byre, 2003;

383   Cuadra *et al*., 2012). Further, the incidence of diffuse and direct radiation is determined at

384   canopy level for near-IR and visible wavelengths (Foley *et al*., 1996; Kucharik *et al*., 2000).

385   Gross C assimilation is then calculated using the approaches described by Farquhar *et al*.

386   (1980) and later simplified and adapted for C4 photosynthesis by Collatz *et al*. (1992). C is

387   then partitioned into stem, root and leaf pools according to variable partitioning parameters

388   within the model: initially, 80%, 10% and 10% of the C assimilated is allocated to the leaf,

389   stem and root pools, respectively, but by the end of the growing season this changes to 10%,

390   80% and 10%, respectively (VanLoocke *et al*., 2010).

391

392   Agro-IBIS contains two major sub-models besides those to simulate land-atmosphere

393   interactions and vegetation dynamics: a belowground C and N module and a solute transfer

394   module. The model represents soil C in three discrete pools and includes both gaseous C

395   losses and those from leaching. These are coupled with N cycling, including four processes to

396   define N availability (Table 1). Soil water availability is controlled by a number of factors

397   including canopy interception, surface runoff and evapotranspiration. Each is calculated for

398   the area based on climate inputs and soil properties with the largest spatially explicit dataset

399   being the limiting factor (Kucharik *et al*., 2000). The model allows for stress from leaf

400   temperature extremes and limited water availability; when given thresholds are exceeded,

401   gross C assimilation and stomatal conductance are modified to simulate the impact of that

402   stress (Mu *et al*., 2007).

403

404 As a DGVM, Agro-IBIS was designed to operate at large spatial scales to predict the impacts

405 of LUC on C budgets but, to date, published simulations are confined to sites in Illinois, USA

406 where good agreement between simulated and observed values for leaf photosynthesis, LAI

407 and latent heat flux were observed (VanLoocke *et al*., 2010). Although the *Miscanthus*-

408 specific values used for parameterising Agro-IBIS have been validated successfully in

409 Illinois, additional field data from a wider range of environmental conditions would ensure

410 that the parameter values used are universal when *Miscanthus* is grown in other locations.

411 Datasets that report LAI, SLA, maximum rubisco activity and measures of maturity in DD

412 would be the most beneficial to verify accompanying yield data given these are key drivers of

413 simulated biomass production. That said, as long as conditions of simulated sites are within

414 the limits of those found at the validated sites in Illinois, the new predictions made by Agro-

415 IBIS are likely to have similar degrees of uncertainty as those reported by VanLoocke *et al*.,

416 2010. Published literature (e.g. Kucharik, 2003; Twine and Kucharik, 2009; Sacks and

417 Kucharik, 2011) for Agro-IBIS has focussed on evaluating its accuracy at simulating

418 harvestable biomass production and a lack of field data has limited verifying model

419 predictions of belowground biomass and soil C sequestration. DGVMs and next generation

420 earth system models such as JULES (Alton *et al*., 2007, Hughes *et al*., 2010) will play an

421 increasingly important part in deciding whether a crop is appropriate for a location, as policy

422 decisions are often based on regions or whole countries, and not individual sites.

423

424 *DayCent*

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426 DayCent is an adaptation of the comprehensive ecosystem model, CENTURY, but with a

427 daily timestep. The DayCent version was originally reported by Parton *et al*. (1998) as a way

428 of producing more reliable simulations of GHG fluxes because they respond rapidly to

429 abiotic factors, and since has been applied to different native and managed systems

430 encompassing a wide range of environmental conditions (Del Grosso *et al*., 2005; Del Grosso

431 *et al*., 2008; Gathany and Burke, 2012). The DayCent model has been calibrated and

432 parameterised for *Miscanthus*, altering N-fixation routines according to the findings by Davis

433 *et al*. (2010). Model outputs from this version of DayCent were verified against

434 measurements in the work. The model does not represent the phenological development

435 stages specific to *Miscanthus* but rather uses a growth response routine according to abiotic

436 factors and water/nutrient availability (Del Grosso *et al*., 2001). This allows DayCent to

437 generate accurate simulations without needing additional inputs about the processes involved

438 in C assimilation.

439

440 NPP is estimated by DayCent according to species-specific relationships of plant growth to

441 soil and air temperature, soil water availability and nutrient availability (Del Grosso *et al*.,

442 2001). For *Miscanthus*, Davis *et al*. (2010) parameterised DayCent using empirical data from

443 Europe and Illinois, USA, (Beale and Long, 1995; Clifton-Brown and Lewandowski, 2000;

444 Heaton *et al*., 2004; Cosentino *et al*., 2007; Heaton *et al*., 2008) to form plant growth

445 parameters. This resulted in simulations being possible in alternate locations where only data

446 for climate and basic soil properties are available (Table 2). Net growth is then partitioned

447 into five plant components (leaves, branches, large wood, fine roots and large roots) as a

448 function of soil water and soil nutrient functions with the most limiting factor (temperature,

449 water, nutrients) having a direct constraint on biomass production (Parton *et al*., 1993). By

450 avoiding measurements of radiation use efficiency (RUE), light extinction coefficient (*k*) and

451 other factors controlling C assimilation, DayCent reduces the number of potentially sensitive

452 parameters that can influence net growth. This simplicity can be considered an advantage

453 over more mechanistic models and because the processes that influence water, nutrient and

454   temperature stress are still represented internally, DayCent remains a fully resolved model

455   when predicting biomass accumulation.

456

457   Separate from the plant production sub-model, DayCent features routines to describe coupled

458   soil water and soil temperature modules, plant decomposition, SOM and trace gas emissions

459   (Table 1). Modelled processes and outputs of DayCent have been validated and verified a

460   number of times since its inception, but Davis *et al*. (2010) reported significant findings

461   regarding additional N-fixation, required when the model was parameterised for *Miscanthus*.

462   These results highlight the importance of a *Miscanthus* model including aspects of the N

463   cycle to ensure the annual demands of the plant are simulated accurately. Following biomass

464   production in the five plant biomass pools, DayCent predicts the amount and quality of plant

465   residue supplemented to the surface and soil, also simulating the plant's influence on the soil

466   environment (Lee *et al*., 2012). This makes DayCent the most comprehensive of the models

467   described here when it comes to C dynamics representing plant and soil interactions. Within

468   the same simulation plant biomass decomposition is calculated, adding C to and transferring

469   C between three conceptual pools in the SOM module: active, slow and passive. Each of

470   these represent different turnover times of the SOM ranging from months and years to

471   centuries and millennia. In addition to these represented C dynamics, nitrogen, phosphorus

472   and sulphur exchange is also cycled through the model, accounting for a number of key

473   processes (Del Grosso *et al*., 2001; Table 1).

474

475   Since CENTURY was developed in the late 1980s, the model or parts of its structure have

476   been used frequently to simulate C and N dynamics, but only recently has the model been

477   parameterised for *Miscanthus*. The only published study validating the *Miscanthus* iteration

478   of DayCent is contained within the inaugural paper and is constrained to field data from

479　Illinois, USA, due to the article's scope (Davis *et al.*, 2010). However, employing the

480　framework and parameter values used by Davis *et al.* (2010), there is no reason why model

481　outputs could not be verified for different plantations at numerous other sites (e.g., those

482　reported in Clifton-Brown *et al.*, 2001a; Danalatos *et al.*, 2007; Christian *et al.*, 2008). Data

483　mining from these studies could prove to be very useful when considering model

484　development, and although the framework of DayCent has been validated numerous times,

485　there is still room for improvement regarding *Miscanthus* simulations (Davis *et al.*, 2010): the

486　models were not initially designed to simulate the nutrient retranslocation from aboveground

487　to belowground plant biomass (e.g. Heaton *et al.*, 2009) that makes *Miscanthus* a particularly

488　attractive bioenergy crop. Similarly, Davis *et al.* (2010) estimated that *Miscanthus* can host

489　N-fixing organisms that can provide up to 25 g N m^{-2} each year - a significant amount for any

490　given land use (Stewart, 1975). Having empirical data to validate this estimate, and the

491　degree of retranslocation, such as the studies by Keymar and Kent (2013) and Heckathorn

492　and DeLucia (1994), respectively, can help model development to ensure simulations are

493　accurate based on specific site conditions.

494

495　*DNDC*

496

497　Originally designed to simulate trace gas emissions and soil C and N dynamics (Li *et al.*,

498　1992), the DNDC model was later calibrated to represent crop growth routines as well as the

499　soils they grow on (named Crop-DNDC; Zhang *et al.*, 2002). More recently, DNDC was

500　parameterised for *Miscanthus* (Borzecka-Walker *et al.*, 2012; Gopalakrishnan *et al.*, 2012).

501　Most aspects of the DNDC model run a daily time step but due to considerable diurnal

502　variation the soil climate and denitrification sub-models operate at hourly time steps. All

503　adaptations of the DNDC model include a plant growth module but the more basic versions

504 simply calculate biomass accumulation according to a generalised crop growth curve using

505 thermal time units. However, the versions parameterised for *Miscanthus* use the mechanistic

506 Crop-DNDC routines allowing crop growth to respond to climatic conditions and soil

507 biogeochemistry. Crop-DNDC simulates crop growth using nine phenological development

508 stages based on those included in CERES models (Ritchie, 1991). Although the original

509 Crop-DNDC structure was applicable for *Miscanthus*, Gopalakrishnan *et al*. (2012) noted the

510 conclusions drawn about N-fixation from Davis *et al*. (2010) and calibrated the DNDC model

511 accordingly, changing the model's default N fixation index from 1 to 3. It is worth noting that

512 within the model, the fixation index is intended to represent N-fixation of the crop directly

513 and not associated organisms, although successful use of this model parameter suggest it may

514 at least help provide accurate yield simulations of *Miscanthus* (Borzecka-Walker *et al*., 2012;

515 Gopalakrishnan *et al*., 2012).

516

517 Crop-DNDC calculates gross photosynthesis using LAI according to Spitters (1986) and

518 gross crop respiration according to McCree (1979) and Penning de Vries *et al*. (1989). The

519 respiration is then subtracted from gross photosynthesis to estimate net C assimilation

520 available for growth. Atmospheric CO_2 concentration, air temperature and the canopy profile

521 are all considered when calculating photosynthetic rates, as are water and nitrogen stress

522 factors (Zhang *et al*., 2002). C is then allocated to stem, leaf, grain and root state variables

523 based on the phonological stage, with more C allocated to stems later in the growing season.

524 Although not initially designed for accurate estimates of crop growth, the adaptations to

525 DNDC now allow accurate simulations after parameterisation using the model's 'Crop

526 Creator' module. Using this module, Gopalakrishnan *et al*. (2012) was able to apply

527 *Miscanthus*-specific parameters to achieve good agreement of model outputs with measured

528 field data. The changed parameters and values used are reported in their paper.

529

530 The DNDC model comprises of six sub-models to simulate crop growth, soil climate,

531 nitrification, denitrification, decomposition and fermentation. Each of these sub-models are

532 coupled so each effects the other and specifically allowing C and N dynamics to be balanced

533 within the system. Although DNDC has most regularly been used to simulate trace gas

534 emissions (e.g. Cai *et al*., 2003; Levy *et al*., 2007; Abdalla *et al*., 2010), the processes

535 governing C dynamics into and between the state variables are equally detailed. Stems, leaves

536 and roots senesced from the crop growth sub-model enter the decomposition sub-model and

537 are allocated to one of three pools: very labile litter, labile litter and resistant litter. The C is

538 moved to microbial and then humad pools before eventually reaching the passive humus

539 pool. For each of these transfers, specific decomposition rates are applied and at each step

540 trace gas emissions are also calculated (Li *et al*., 1994; Li, 2000).

541

542 The DNDC model has been used frequently since its inception but only recently has the

543 model been parameterised and tested to simulate the C and N dynamics of a *Miscanthus*

544 plantation. There are two publications reporting DNDC used to simulate *Miscanthus* growth

545 but both focus mainly on the nitrogen losses and trace gas emissions associated (Borzecka-

546 Walker *et al*., 2012; Gopalakrishnan *et al*., 2012). Consequently it is difficult to review the

547 model performance for ecosystem C budgets, but both papers report good agreement between

548 modelled and measured values of crop yield. Confidence in this agreement can also be drawn

549 from the different locations simulated; the Gopalakrishnan *et al*. (2012) paper simulated

550 yields in Illinois, USA, whereas Borzecka-Walker *et al*. (2012) simulated *Miscanthus*

551 plantations in Poland, where annual precipitation was roughly half that of the sites in Illinois.

552 The DNDC model represents soil processes mechanistically and in a lot of depth, and is

553 therefore particularly good at improving our understanding of how *Miscanthus* plantations

554 may influence key issues regarding the crop's sustainability criteria (e.g. net change in soil C,

555 GHG emissions and N dynamics). Each of these were simulated and reported by Borzecka-

556 Walker *et al.* (2012) with interesting results that suggest soil type has a significant impact on

557 potential soil C storage, net global warming potential and soil N balance, but not on yield.

558 However, these simulations were only valid for the site modelled as there is not sufficient

559 field data to initialise the model at different *Miscanthus* sites. The model requires inputs of

560 each of the SOM pools in kg C kg^{-1} soil and few datasets include this information; soil

561 fractionation to relate measured soil C fractions to conceptual modelled pools is a relatively

562 recent aspect of this research. However as fractionation data becomes more readily available,

563 DNDC's SOM module outputs can be validated for a range of sites and conditions with

564 added confidence given the successful simulations performed by Borzecka-Walker *et al.*

565 (2012). An additional aspect of the DNDC model that makes it particularly attractive is its

566 integration with GIS databases (e.g. Pathak *et al.*, 2005; Tang *et al.*, 2006). This allows many

567 of the model outputs to be scaled up across larger regions as long as there is sufficient high

568 quality input data to drive the simulations.

569

570 *ECOSSE*

571

572 The ECOSSE model (Smith *et al.*, 2010a) was developed to simulate highly organic soils

573 from concepts originally derived for mineral soils in the RothC (Jenkinson and Rayner, 1977;

574 Jenkinson *et al.* 1987; Coleman and Jenkinson, 1996) and SUNDIAL (Bradbury *et al.* 1993;

575 Smith *et al.* 1996) models. Following these established models, ECOSSE is primarily

576 designed to simulate belowground C and N dynamics but has more recently been coupled

577 with an updated version of the MIAMI model (Leith, 1972) to calculate NPP. ECOSSE uses

578 a pool type approach, describing soil organic matter (SOM) as pools of inert organic matter

579   (IOM), humus (HUM), biomass (BIO), resistant plant material (RPM) and decomposable

580   plant material (DPM). All of the major processes of C and N turnover in the soil are included

581   in the model, but each of the processes is simulated using only simple equations driven by

582   readily available input variables, allowing it to be developed from a field based model to a

583   national scale tool, without high loss of accuracy. ECOSSE differs from RothC and

584   SUNDIAL in the addition of descriptions of a number of processes and impacts that are

585   important in organic soils, but not relevant in the mineral arable soils that these models were

586   originally developed for. More importantly, ECOSSE differs from RothC and SUNDIAL in

587   the way that it makes full use of the limited information that is available to run models at

588   national scale. In particular, measurements of soil C are used to interpolate the activity of the

589   SOM and the plant inputs needed to achieve those measurements. Any data available

590   describing soil water, plant inputs, nutrient applications and timing of management

591   operations are used to drive the model and so better apportion the factors determining the

592   interpolated activity of the SOM. However, if any of this information is missing, the model

593   can still provide accurate simulations of SOM turnover, although the impact of changes in

594   conditions will be estimated with less accuracy due to the reduced detail of the inputs (Smith

595   *et al.*, 2010b).

596

597   The total plant inputs of C are assumed to be given by the NPP. If this is known, it can be

598   entered as an input by the user, otherwise, NPP is entered as zero and the plant inputs are

599   estimated using the MIAMI model (Leith, 1972). The N inputs from the plant to the soil are

600   calculated using standard C:N ratios for the different land uses. The C:N ratios of simple land

601   use classes, such as arable, grassland, forestry and semi-natural, are initially all set to 10. As

602   an alternative, in the site specific version of the model, the plant inputs of C and N can be

603   calculated from the expected yield as described by Bradbury *et al.* (1993). The plant input of

24

604 C is given as a function of the crop yield modified by empirical parameters, specific to each

605 crop or plant type. The plant input of N is calculated from the amount of N taken up in above

606 ground plant biomass.

607

608 The rates of decomposition modelled by ECOSSE are important determinants in the

609 modelling of soil N and N_2O emissions, as the soil N content follows the decomposition of

610 SOM (Bell *et al*., 2012). The rate of SOM decomposition in the model is modified by

611 temperature, soil water content, plant cover and soil pH. Decomposition rate is also

612 dependent on how SOM is proportioned into the different SOM pools. Following the

613 approach used in the RothC model (Coleman and Jenkinson, 1996), the IOM pool does not

614 undergo decomposition; the C in this pool does not take part in soil processes either due to its

615 inert chemical composition or its protected physical state. The HUM pool decomposes

616 slowly, representing material that has undergone stabilization due to earlier decomposition

617 processes. The BIO pool decomposes more rapidly and represents material that has

618 undergone some decomposition but is still biologically active. The DPM and RPM pools are

619 composed of undecomposed plant material, the DPM pool being readily decomposable while

620 the RPM pool is more recalcitrant. The ratio of DPM to RPM defines the decomposability of

621 the plant material that is added to the soil. Values for the ratio of DPM to RPM for the

622 different land uses are standard as used in RothC, although these can be changed within

623 ECOSSE for a specific instance of a land use type (e.g. *Miscanthus*).

624

625 In ECOSSE, soil layers are divided into 5 cm layers. Each layer is filled with water until it

626 reaches field capacity, when it then drains to the layer below, or evaporates from the

627 uppermost layer. ECOSSE differs from many other soil models, as it is able to simulate how

628 decomposition will respond to soil water contents above field capacity. The model assumes

629   that decomposition is at its maximum at field capacity, but is slowed by water limitation

630   below field capacity, and oxygen limitation above field capacity. When the water content is

631   above field capacity the decomposition rate falls linearly, and at saturation it is only 20% of

632   that at field capacity (Smith *et al*., 2010a). Under aerobic conditions, the decomposition

633   process results in gaseous losses of CO_2; under anaerobic conditions losses as methane (CH_4)

634   dominate. The N content of the soil follows the decomposition of the SOM, with a stable C:N

635   ratio defined for each pool at a given pH, and N being either mineralised or immobilised to

636   maintain that ratio. Nitrogen released from decomposing SOM as ammonium (NH^{4+}) or

637   added to the soil may be nitrified to nitrate (NO^{3-}). C and N may be lost from the soil by the

638   processes of leaching (NO^{3-}, dissolved organic C (DOC), and dissolved organic N (DON)),

639   denitrification, volatilisation or crop offtake, or C and N may be returned to the soil by plant

640   inputs, inorganic fertilizers, atmospheric deposition or organic amendments.

641

642   The ECOSSE model has already been validated and applied spatially to simulate land-use

643   change impacts on SOC and GHG emissions (Smith *et al*., 2010a,b) and to simulate soil N

644   and N_2O emissions in cropland sites in Europe (Bell *et al*., 2012). Smith *et al*. (2010a,b)

645   reported the estimate in Scottish soil C stocks and changes using ECOSSE. The results of this

646   work reported that, despite the uncertainties in the input data and the measurements used to

647   evaluate the model, the simulated values show a high degree of association with the

648   measurements in both total C and change in C content of the soil. Over all sites where land-

649   use change occurred, the average deviation between the simulated and measured values of

650   percentage change in soil C was less than the experimental error (11% simulation error, 53%

651   measurement error). This suggests that the uncertainty in using this model for the national-

652   scale simulations will be ~11%. Bell *et al*. (2012) reported the first test of the ECOSSE

653   model at predicting N_2O emissions from arable soils in Europe, indicating that although

654 further modifications are required in the form of predictions on a daily time-step, the model is

655 currently predicting such fluxes with a greater degree of accuracy than other available

656 methods of quantification which can then be used to estimate emissions on a large scale. The

657 parameterisation and evaluation of ECOSSE to simulate soil C and GHG emissions under

658 *Miscanthus* and short-rotation forestry is currently on-going and the results are in preparation

659 for publication.

660

661 **Alternatives to mechanistic crop models**

662

663 In addition to the models that fulfil our original selection criteria there are other relevant

664 models which satisfy a subset of our criteria. Alternatives include empirical models (Heaton

665 *et al*., 2004; Richter *et al*., 2008), soil-only models (Dondini *et al*., 2009), plant growth only

666 models with no soil C components (Clifton-Brown *et al*., 2000; Hastings *et al*., 2009a) and

667 those where no peer-reviewed literature exists supporting the models' validities for

668 *Miscanthus* specifically (e.g. EPIC (Williams *et al*., 1989) reported by Zhang *et al*. (2011)

669 and JULES (Hughes *et al*., 2010).

670

671 Empirical models are excellent simple predictors when estimating how a known set of

672 conditions will influence a specific variable, and are likely to provide more accurate

673 predictions than mechanistic alternatives, since they are built solely around field observations

674 and not the biogeochemical processes that define plant growth or C transfer. However, this

675 also means empirical models require a large amount of field data from individual sites, and

676 their simulations cannot be used to predict the system's response to environmental variation.

677 Heaton *et al*. (2004) and Richter *et al*. (2008) used observed *Miscanthus* yields and

678 accompanying site conditions (i.e., soil type, growing degree days, average precipitation) to

679   create empirical models capable of simulating different scenarios of available N, air

680   temperature and water availability. Their model outputs correlated well with observed values

681   and using known site conditions across larger spatial areas each was able to predict potential

682   yields and how they would be affected by changes in N-availability, air temperature and

683   water availability. While informative for this purpose, the models are less suitable for

684   understanding why yields vary. Furthermore, creating similar empirical models to simulate

685   the response of other variables of interest (e.g. soil C) is unlikely to be successful, due to the

686   number of factors that drive change in those variables and the lack of field data for

687   *Miscanthus*.

688

689   Soil-only models that describe the belowground C dynamics of *Miscanthus* plantations can

690   predict changes to soil C stocks over time but by definition do not include any plant growth

691   routines and so lack information when considering the total ecosystem C budgets. Primarily,

692   RothC (Coleman and Jenkinson, 1999) has been the chosen model to simulate soil C

693   dynamics beneath *Miscanthus* plantations (Dondini *et al*., 2009; Hillier *et al*., 2009; Poeplau

694   and Don, 2013). This process-based model is similar to the SOC sub-models included in

695   DayCent, WIMOVAC, BioCro and Agro-IBIS, and like these models, their outputs come

696   with considerable uncertainty due to limited validation data for *Miscanthus* plantations under

697   a wide range of environmental conditions. That said, the work done by Dondini *et al*. (2009)

698   and Poeplau and Don (2013) is taking great steps to help reduce the associated uncertainty

699   and continued investigation into the size of measurable soil C pools using fractionation

700   techniques will provide the information regarding initial pool sizes that is essential for

701   accurate simulations of soil C dynamics.

702

703   Just as soil-only models do not include plant-growth routines, models like MISCANMOD

704   (Clifton-Brown *et al*., 2000) and MISCANFOR (Hastings *et al*., 2009a) do not include sub-

705   models to describe soil C dynamics. Both MISCANMOD and MISCANFOR have been used

706   to simulate *Miscanthus* productivity across the UK and Europe using a number of databases

707   for required inputs (Clifton-Brown *et al*., 2004; Hastings *et al*., 2009b; Pogson *et al*., 2012).

708   More recently, MISCANFOR was also used to predict *Miscanthus* yields globally and relate

709   them to potential energy generation accounting for land use, cost and carbon restrictions

710   (Pogson *et al*., 2013). The crop growth routines used in these *Miscanthus*-specific models

711   have regularly been proven to be accurate within a wide range of environmental conditions

712   but the model's lack of soil C pools make it of limited use when requiring information about

713   the full ecosystem C budget. Consequently, coupling such models with those that describe

714   other aspects of the C cycle may allow for accurate simulations without developing a whole

715   new model.

716

717   The EPIC model (Williams *et al*., 1989) is a mechanistic model that is reported to have been

718   parameterised for *Miscanthus* and showed a good correlation between field data and model

719   output (Zhang *et al*., 2011). However, no further detail is given by the Zhang *et al*. (2011)

720   paper. Similarly the JULES model (Met Office, 2013) was used by Hughes *et al*. (2010) to

721   simulate *Miscanthus* production and calculate payback times for different regions globally,

722   based on the assumption that 50% of NPP is available to offset fossil fuel emissions. The

723   JULES model is essentially a land-atmosphere energy transfer model but it includes

724   TRIFFID, a DGVM much like Agro-IBIS. Although the Hughes *et al*. (2010) study reports

725   parameterisation of the JULES simulation, and the values used, there is no discussion of its

726   validation against field data. Therefore the reliability of its predictions cannot be assessed or

727   the uncertainty quantified. That said, the study integrates the JULES model with the global

climate impacts model, IMOGEN, to simulate the impact of IPCC Special Report Emissions

Scenarios (Hughes *et al*., 2010). After validation from field data encompassing a range of

environmental conditions, this is the right approach to predicting how beneficial *Miscanthus*

plantations may be in different regions.

A simple semi-mechanistic model created to estimate C sequestration rates under *Miscanthus*

plantations was reported by Matthews and Grogan (2001) over a decade ago but has not since

been further developed. The model by Matthews and Grogan (2001) uses solar radiation, the

light extinction coefficient (k) and LAI to estimate biomass production and partitions this

according to the values reported by Himken *et al*. (1997). In this way it is very similar to a

number of mechanistic models that have been developed for bioenergy crops since (see

Surendran Nair *et al*., 2012). Each of the plant and soil values required to parameterise

Matthews and Grogan's model were taken from published field data and decomposition was

estimated using decay rates that adhere to first-order kinetics. The model was based on mass-

balance principles but did not have data from a *Miscanthus* plantation to verify its

predictions. Instead, it used parameters specific to a woodland site to verify outputs against

field data, reporting a good correlation between observed and simulated values. Since the

model does not include environmental variables such as precipitation or air temperature, it is

not capable of simulating different climatic scenarios. However, if model predictions can be

verified, a sensitivity analysis could reveal how changing LAI or the proportion of plant

biomass allocated belowground (i.e. changes that may occur in genetic variants) may impact

soil C sequestration rates.

Future modelling of *Miscanthus* plantations

752

753 **Empirical data beneficial for improving model performance**

754

755 Each of the models described have their own advantages and disadvantages dependent on the

756 research objective, input data availability and the required outputs (at appropriate temporal

757 and spatial scales). Overall, there is an increasing number of datasets becoming available to

758 aid model improvement, inter-model comparisons and uncertainty quantification. That said,

759 certain aspects of the *Miscanthus* C cycle remain poorly quantified due to a lack of

760 experimental data and in particular, parameters describing belowground biomass and root

761 turnover. These scarcely-quantified model parameters are the crux of defining how much C is

762 sequestered in the soil and also of changes in stable soil C stocks that can help offset the C

763 emissions associated with energy generation from *Miscanthus* biomass. Another important

764 area which requires attention relates to the assigned splitting ratios in SOM modules. These

765 dictate how much C is allocated to the stable or labile soil pools, which in turn determines

766 how long the C is predicted to stay in the soil. To relate these conceptual labile or stable

767 pools of C used by the models to measurable pools, soil fractionation is possible using

768 physiochemical procedures, such as that suggested by Zimmermann *et al*. (2007). To date

769 there are only two published studies relating soils beneath *Miscanthus* plantations to SOM

770 pools (Dondini *et al*., 2009; Poeplau and Don., 2013). Both studies suggest that an increase in

771 total SOC during the lifetime of a *Miscanthus* plantation is likely, but their estimates of

772 change in stable soil C pools vary considerably. If full C accounting is desired to satisfy

773 cradle-to-grave life-cycle analyses (LCAs) it is essential to accurately predict soil C

774 sequestration rates using stable isotope techniques as used by Dondini *et al*. (2009) and

775 Poeplau and Don (2013).

776

777   Validating model predictions has principally been achieved through comparison with young

778   commercial *Miscanthus* plantations (e.g. Case *et al*., 2013; Zimmermann *et al*., 2013) or field

779   trials (e.g. Christian *et al*., 2008; Borzecka-Walker *et al*., 2012). However these do not

780   address issues of optimal crop rotation length, nor do they necessarily reflect the same site

781   conditions experienced by an old (10+ years) commercial plantation of considerable size.

782   This is particularly true for field trials where continued disturbance and different plant

783   densities can influence final yield (Lewandowski *et al*., 2000; Lewandowski *et al*., 2003b).

784   Consequently, the importance of continuing to monitor existing commercial plantations

785   cannot be underestimated if we are to ensure model predictions are accurate throughout the

786   entire lifecycle of a *Miscanthus* plantation. The few larger and older plantations that have

787   been studied indicate that yields can vary greatly depending on climatic conditions during

788   each year and that *Miscanthus* plantation yields become less commercially viable after 20

789   years of continual harvesting (Clifton-Brown *et al*., 2001b; Khanna *et al*., 2008). It is

790   therefore reasonable to assume other aspects of the C cycle (i.e. soil C sequestration and

791   GHG emissions) may be interacted upon by changes in crop productivity. Since *Miscanthus*

792   is a relatively recent addition to land owner's establishment options there are few studies in

793   Europe or North America that report how the LUC to a commercial sized plantation affects

794   the site's C budgets (e.g. Zimmermann *et al*., 2012). To ensure the mechanistic relationships

795   represented by the model simulations are accurate for the LUC and management for both

796   normal and extreme conditions, we need additional field data.

797

798   **Databases and frameworks for *Miscanthus* model development**

799

32

800　Comprehensive datasets from single field sites are needed to 1) better quantify model

801　uncertainty and 2) allow for model comparison. With the advances in database technology

802　and ease of electronic communication for data sharing, such exchanges are becoming more

803　achievable and recently online databases have been created (e.g. LeBauer *et al*., 2010).

804　Sensitivity and uncertainty analyses of the models can help identify where data collection

805　needs focus to best reduce uncertainty; however, for all process-based models, uncertainty

806　can come from inputs, model structure or observations (Smith *et al*., 2012a). Due to the

807　number of sources of uncertainty and limited data availability at present, uncertainty

808　quantification is rarely addressed by the literature that report *Miscanthus* simulations. That

809　said, LeBauer *et al*. (2013) were able to provide estimates of how much model uncertainty is

810　due to individual model parameter values by using a Bayesian meta-analysis with available

811　species-specific data. Although, their study uses the specific example of switchgrass, the tool

812　they report and use (the Predictive Ecosystem Analyzer; PEcAn) is just as applicable to

813　*Miscanthus*. PEcAn can therefore be used with the six models reported here to identify which

814　model parameters contribute most to uncertainty, providing much more information than

815　simple sensitivity analyses.

816

817　In addition to data availability limiting model development, a comprehensive framework is

818　lacking around which the different crop models can be developed from site-scales up to

819　regional, or even continental, scales. This is arguably the most important aspect of future

820　model development, since model outputs are the best predictions we have to inform policy

821　decisions. Since governmental policies are often a major driver of LUC, and occur over large

822　geographical scales, a key requirement before *Miscanthus* plantations are established is the

823　implementation of an integrative computational framework (Zhang *et al*., 2010). This

824　framework should 1) compile comparable, and spatially explicit, input data; 2) execute model

825 simulations and report outputs that are consistent with each other; 3) prepare unambiguous

826 visualisations of the findings. Surendran Nair *et al*. (2012) suggest that such a framework

827 should include a GIS for reprocessing spatial datasets (e.g., Zhang *et al*., 2010) and an

828 efficient platform upon which to perform model simulations and powerful post-processing

829 analysis of model predictions (e.g., Nichols *et al*., 2011) — thereby allowing simple

830 comparisons between biomass production/C dynamics and geographic features/climate data

831 to be visualised. Model adaptations of MISCANFOR to simulate *Miscanthus* biomass

832 production over GIS datasets for Europe (Pogson, 2011; Pogson *et al*., 2012) and globally

833 (Pogson et al., 2013) are good examples of how upscaling existing models may be the fastest

834 way of forming reliable predictions over larger spatial areas. Similarly, it is worth specifically

835 mentioning the framework outlined by Zhang *et al*. (2010). This was able to extract input

836 information from text files for use in the EPIC model (Williams *et al*., 1989) and overlay

837 results against GIS maps. Validated outputs from simulations running under frameworks such

838 as this are promising indicators of how model development may progress in the near future.

839

840 Implementing an ecosystem model over large geo-spatial regions requires the most

841 appropriate input databases for site characteristics, such as soil type and climatic variables.

842 Most ecosystem models use similar driving data. Recent applications of *Miscanthus* models

843 at UK (Hastings *et al.*, 2013), European (Hastings *et al.*, 2009) and global levels (Pogson *et*

844 *al.*, 2013) demonstrate that appropriate datasets exist at a range of spatial scales to run energy

845 crop soil models. Smith *et al.*, (2012b) recently reviewed spatial datasets available for

846 modelling soil C change at regional to global scales.

Conclusions

In the coming years, a drive toward renewable sources of energy and commitments to reduce national CO_2 emissions are likely to increase interest in bioenergy crops such as *Miscanthus*, and therefore may induce considerable LUC around the world. With land resources diminishing and concerns for food security increasing, it is a major concern that any LUC that does occur is appropriate and the most effective land use for a given area. Process-based models are valuable tools for addressing this issue and it is therefore essential that they operate reliably for a wide range of environmental conditions. Here we reviewed six process-based crop models that have been parameterised for *Miscanthus*, reported the current extent of their application and described the possible uses of these models. The models differ in both their design and computational power but none is vastly superior; selecting one over another depends mainly on the particular research question to be answered.

For model development to occur, and therefore to improve the reliability of model predictions, high-quality experimental field data are essential. As interest has grown in the viability of *Miscanthus* as a bioenergy crop, experimental data from its non-native countries has increased considerably, but not all is freely available or accompanied by the supporting information essential for model development. In addition, to better validate the internal model parameters and rate modifiers, increased data availability through data sharing is also key to addressing the issues of uncertainty quantification and model comparisons, which is necessary for ensuring realistic model outputs. The scientific modelling community is sufficiently motivated to develop *Miscanthus* crop models and therefore it is highly likely that as data availability and computational modelling power increases, there will be a significant improvement in *Miscanthus* model performance.

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Table 1: Model characteristics, submodels and components of six crop growth models parameterised for *Miscanthus* (format adapted from Surendran Nair *et al*. (2012) to aid comparison between the papers).

Model	Spatial Scale	Biomass Production Submodel			Hydrological Submodel	Soil Quality Submodel			Stress factors	
		Phenological development	Biomass calculation method	Biomass partitioning	Processes simulated	Carbon losses simulated	SOC pools represented	Nitrogen processes simulated	Factor considered	Variables affected
WIMOVAC and BioCro	Site/Ecosystem	6 stages	Biochem.	4 pools	R, Et	G, L	A, S, P	Min, Imm	W	Stomatal conductance
Agro-IBIS	Ecosystem	3 stages	Biochem.	3 pools	C, R, Et	G, L	A, S, I	Min, D, N, Le	W, NL	Photosynthesis
DAYCENT	Site	Curve	ARF	5 pools	C, Et, Sf	G, E, L, F	Mic, A, S, P	Min, Imm, D, N, V, Le	W, T, NL, O	Element budgets
DNDC	Site	Curve / 9 stages*	Biochem.	4 pools	C, R, Et	G, L	Res, Mic, H, P	Min, Imm, D, N, V, Le	W, NL	Biomass, Partitioning, Nitrogen budgets
ECOSSE	Site/Regional	Curve	Biochem.	5 pools	R, Et	G, L	A, S, P, I, Res, H	Min, Imm, D, N, V, Le	W, T, NL, O	Partitioning, Nitrogen budgets, Carbon budgets

* Depending on version of the model. RUE - Radiation Use Efficiency, Biochem. - Biochemical approach, ARF - Abiotic Response Function C - Canopy interception, R - Runoff, Et - Evapotranspiration, Sf – Storm Flow, G - Gaseous, E - Erosion, L - Leaching, F - Fire, Mic - Microbial Biomass, S - Slow, P - Passive, A - Active, I - Intermediate, Res - Residual plant litter (very labile, labile and resistant), H - Humads (labile and resistant), Min - Mineralisation, Imm - Immobilization, D - Denitrification, N - Nitrification, Le - Leaching, V - Ammonium volatilization, W – Water limitation, T – Temperature limitation, O - Oxygen limitation, NL - Nutrient limitation, LAI - Leaf Area Index, Element Budgets - Includes carbon, nitrogen, phosphorus and sulphur.

Table 2: Essential and optional input parameters required by six process-based carbon models parameterised for *Miscanthus*.

Model	Essential input parameters			Optional input parameters
	Weather input parameters	Site input parameters	Crop input parameters	
WIMOVAC and BioCro	Air temperature Solar radiation Relative humidity Wind speed Precipitation	Sand, silt and clay contents Initial soil C pools Soil pH Latitude and altitude Field capacity Wilting point Irrigation, sowing, harvest dates	Maximum rooting depth Maximum carboxylation rate Quantum efficiency Dark respiration Thermal periods for growth stages Dry matter partitioning coefficients	Parameters easily changed through *R* function calls (generic WIMOVAC model has user interface front end) Rate and timing of fertiliser application Tillage timing and technique
Agro-IBIS	Air temperature Solar radiation Relative humidity Wind speed Precipitation	Sand, silt and clay contents Initial soil C pools for all layers Soil pH Soil bulk density Initial soil C pools Irrigation, sowing, harvest dates	Maximum carboxylation rate Quantum efficiency Dark respiration	Additional climate inputs (e.g. days frost per year) edited via text file inputs Rate and timing of fertiliser application Tillage timing and technique
DAYCENT	Max./Min. Air Temperature Precipitation	Sand, silt and clay contents Soil pH Initial soil C pools for all layers Latitude and longitude	Respiration partitioning coefficients Biomass partitioning coefficients Crop growth temperature thresholds Thermal periods for growth stages N and lignin content	Relative humidity and wind speed Soil C for each 15 cm layer Rate and timing of fertiliser application Tillage timing and technique Water and nutrient stress modifiers Solar radiation
DNDC	Max./Min. Air temperature Precipitation N rainfall concentration	Sand, silt and clay content Soil pH Soil bulk density Initial soil C pools Initial NO_3^-/NH_4^+ soil contents Latitude, longitude and slope	Leaf area index Maximum crop height Thermal degree days Biomass partitioning coefficients Thermal periods for growth stages	Atmospheric CO_2 & NH_3 concentrations Rate and timing of fertiliser application Tillage and harvest timings Soil C for each 5 cm layer Solar radiation
ECOSSE	Air temperature Potential evapotranspiration Precipitation	Sand, silt and clay contents Initial soil C Soil pH Soil bulk density Water Table depth Latitude	Vegetation cover type (*Miscanthus* parameters are already included within the basic version)	Rate and timing of fertiliser application Annual crop yield Tillage and harvest timings Soil C for each 5 cm layer Solar radiation