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Supporting Information (SI)

Environmental Life Cycle Assessment of producing willow, alfalfa and straw from spring barley as feedstocks for bioenergy or biorefinery systems

Ranjan Parajuli[a,*], Marie Trydeman Knudsen[a], Sylvestre Njakou Djomo[a], Andrea Corona[b], Morten Birkved[b], Tommy Dalgaard[a]

[a]Department of Agroecology, Aarhus University, Blichers Allé 20, DK-8830 Tjele, Denmark

[b]Department of Management Engineering, Technical University of Denmark, Building 424, DK-2800 Lyngby, Denmark

[*]Corresponding author, email: ranjan.parajuli@agro.au.dk, Phone: +4571606831

Contents

S1. Calculation of non-harvestable residues for alfalfa

To calculate the SOC change for alfalfa, required parameters were taken averaging from the two studies Djurhuus and Hansen (2003) and Pietsch *et al.* (2007). The consistency of the assumed parameters (Table S.1) were checked with Taghizadeh-Toosi *et al.* (2014a), and was further compared with the dataset of C-tool (Petersen *et al.*, 2013).

Table S.1: Required parameters for alfalfa to calculate the non-harvestable residues and related C assimilation (values indicated as C= calculated, M = measured, A = assumed) after the given references

Parameters/Sources	Unit	Calculated after, (Djurhuus and Hansen, 2003)	Calculated after, (Pietsch et al., 2007)	Average
a. Above ground biomass removed	t DM/ha	12.2 (C)	8.68 (M)	10.44
b. Total root biomass[1]	t DM/ha	2.68 (C)	2.26 (C)	2.68
c. Root + stubble	t DM/ha	4.85 (M)	5.75 (M)	5.3
d. Stubble only	t DM/ha	2.17 (M)	3.49 (M)	2.83
e. Senescence	t DM/ha	1 (M)	1 (A)	1
f. Stubble/(harvested yield)		0.18 (C)	0.4 (C)	0.29 (C)
Harvest index of main crop relative to aboveground biomass (alfa)[2]	ratio	0.79 (C)	0.66 (C)	0.53
Root and exudate C as proportion of total C assimilation (beta), root of total fixed C[3]		0.26 (C)	0.26[†] (C)	0.26
Stubble + root/net yield[4]		0.4 (C)	0.66 (8C)	0.53

Assumptions:

[1] Calculated from the above data sets (c-d)

[2] Calculated from above data sets [a/(a+d+e)].

[3] Calculated based on the ratio of root DM (Djurhuus and Hansen, 2003) to the net yield.

[†] calculated accordingly assuming the root DM as in Djurhuus and Hansen (2003).

[4] Calculated from above data sets (c /a).

S.2. Calculation of the SOC change according to IPCC method

In the basic scenario (Table 2), SOC change in 20 years and 100 years were calculated based on the method suggested in Petersen et al. (2013). In the sensitivity analysis, the calculation is based on the IPCC Tier 1 methodology (IPCC, 2006), modified in Grogan and Matthews (2002). SOC available from the non-harvestable above ground and below ground residues were calculated for the production of selected crops and the reference crop land (Eq. i). Available SOC from the below and above ground residues for the main crop (C_{BGmi} and C_{AGmi} respectively) and from the reference crop (C_{BGr} and C_{AGr}) are shown in Table 2 of the main document.

$$\Delta GHG_{SOC} = \left[\frac{(C_{BGr} - C_{BGmi}) + (C_{AGr} - C_{AGmi}) + SOC_{ini} * F_{mg} * F_{I} * (F_{LUr} - F_{LUmi})}{(Y_{mi} * T)} \right] * 3.66$$

............................Eq. (i)

where, initial SOC stock (SOC_{ini}) = 90 t C/ha (Taghizadeh-Toosi *et al.*, 2014b), F_{MG} and F_{I} are the relative stock change factors related to the management and inputs (IPCC, 2006). Relative stock change factors for the reference land use and the main crop production indicated over 20 years were adapted from IPCC (2006). The reference land use was assumed, as was continuously managed by annual crops for greater than 20 years (IPCC, 2006). Y_{mi} (t DM/ha/y) is the annual yield of the biomasses (Table 2, in the main document). A negative value of ΔGHG_{SOC} implies a carbon sink where as a positive value represents a source for GHG emissions In the case of barley the impact related to agricultural residues removal was also calculated from equation (ii) and was added to the equation (i).

$$\Delta GHG_{residues} = \left[\frac{SOC_{ini} * F_{mg} * F_{LUmi} * (F_{INr} - F_{IR})}{(Y_{m_i} * T)} \right] * 3.66$$

............................Eq. (i)

where, SOC_{ini} = initial SOC stock; F_{LU} and F_{MG} are the relative stock change factors related to land use and management. F_{IN} and F_{IR} are the relative stock change factors related to inputs under no residues removal and their removal respectively (IPCC, 2006). T=20 years is the accounting period, and 3.66 is the ratio of the molecular weight of CO_2 to C. Related parameters are shown in Table S.2.

Table S.2. Relative stocks change factors related to the land use and management over 20 years, adapted from IPCC (2006)

Parameters/Crops	Spring barley	Willow	Alfalfa
Accounting period (T)	20	20	20
Yield (Y_m)	3.94	10.63	12.204
Factors assumed:			
- Initial Soil C (C_o)	90	90	90
- Reference land use[a] (F_{LUr})	0.69	0.69	0.69
- Main crop$_1$ (F_{LUm})	0.69[a]	0.82[b]	0.82[b]
- Tillage[c] (F_{mg})	1	1	1
- Input (F_I)	0.92[d]	1.11 [e]	1 [f]
Factors assumed for residues:			
- Straw residues removed (F_R)	0.92	-	-
- Straw residues incorporated F($_{in}$)	1	-	-

Assumptions:

[a] Area continuously managed for >20 yrs, to predominantly annual crops.

[b] Relative change of SOC stock for temporary set aside of annually cropland.

[c] Full tillage

[d] low residues return.

[e] High residue return without manure.

[f] Medium residue return.

S3. Inventory for willow-cuttings production

The database for the willow-cuttings production was based on the annual average material inputs assumed for the production of willow during the period of the plantation until the first harvest. The inputs estimated per 1 ha of land (Table 1 in the main document) was assumed for the production of about 300,000 cuttings (Sevel *et al.*, 2012). The numbers of cuttings assumed for the plantation in 1 ha of land was 12,000 (Hamelin *et al.*, 2012; Sevel et al., 2012).

Table S.3. Inventory for the willow cuttings production

Activities	Units	Input per ha[1]	Remarks
a. Direct primary energy input (diesel)[2]			
Ploughing	MJ/ha/y	35	Diesel = 20.7 l/ha
Rotary harrowing	MJ/ha/y	8	Diesel = 4.76 l/ha
Fertilizing	MJ/ha/y	45	Diesel = 2 l/ha
weed control	MJ/ha/y	10	Diesel = 1.5 l/ha
Whip harvester, diesel	MJ/ha/y	156	Diesel= 90.85 l/ha
b. Agro-chemicals input			
N	kg/ha/y	74	Table 1
P	kg/ha/y	73	Table 1
K	kg/ha/y	207	Table 1
Glyphosate + other herbicides	kg/ha/y	1.036	Table 1
c. Transport of cuttings[3]	t km	d. 0.72	

Assumptions:

[1] Based on the annual input considered for the willow production until the first harvest (Table 1).

[2] Norms of diesel input was based on Dalgaard *et al.* (2001)· ± Diesel for willow-cuttings harvest was based on Caputo *et al.* (2013).

[3] Transport of willow-cuttings as the plantation. Weight of cuttings = 20 g/cuttings (Rewald *et al.*, 2016) at 3 km distance.

S4. List of active ingredients assumed for the production of the selected crops

The active ingredients of the pesticides, as shown in Table S.4 were the total doze applied 1 ha of land for the production of the selected crops (Ørum and Samsøe-Petersen, 2014; SEGES, 2010). The annual average doze, as presented in the main analysis (Table 1) was calculated after dividing by the respective life cycle years of the selected crops production.

Table S.4. List of pesticides and total doze applied over the life cycle years of the selected crops **(**Herbicides = H, Growth regulator= G, Fungicides = F and Insecticides = I)

Pesticides, a.is.	Types	CAS	Application (kg/ha)[1]		
			Spring barley[±]	Alfalfa[±±]	Willow[±±]
2,4-d	H	94-75-7	0.0052	-	-
Bentazone	H	25057-89-0	0.0202	0.479	-
Aminopyralid	H	150114-71-9	0.0002	-	-
Bromoxynil	H	1689-84-5	0.0355		-
Clodinafop-propargyl	H	105512-06-9	0.00002	-	-
Clopyralid	H	1702-17-6	-	-	0.031
Cycloxydim	H	101 205-02-1	-	-	0.286
Dicamba	H	83164-33-4	0.0007	-	-
Diflufenican	H	71283-80-2	0.0070	-	0.0476
Fenoxaprop-p-ethyle	H	145701-23-1	0.0058	0.069	-
Florasulam	H	144740-54-5	0.0003	-	-
Foramsulfuron	H	173159-57-4	-	-	19.048
Fluroxypyr	H	69377-81-7	0.0207	-	-
Glyphosate	H	1071-83-6	-	-	-
Iodosulfuron-methyl-natrium	H	144550-36-7	0.0006	-	-
Ioxynil	H	1689-83-4	0.0324	-	-
MCPA	H	94-74-6	0.2448	-	-
Metsulfuron-methyl	H	74223-64-6	0.0003	-	-

Pendimethalin	H	40487-42-1	0.0119	0.45	0.19
Propaquizafop	H	111479-05-1	-	-	0.095
Triasulfuron	H	52888-80-9	0.00003	-	-
Tribenuron-methyl	H	400852-66-6	0.0021	-	-
Sulfosulfuron	H	141776-32-1	0.00002	-	-
Thifensulfuron-methyl	H	79277-27-3	0.0002	-	-
Chlormequat-chlorid	G	104206-82-8	0.0110	-	-
Ethephon	G	101-21-3	0.0257	-	-
Mepiquat-chlorid	G	1596-84-5	0.0037	-	-
Prohexadion-calcium	G	16672-87-0	0.00004	-	-
Trinexapac-ethyle	G	56425-91-3	0.0025	-	-
Azoxystrobin	F	131860-33-8	0.0016	-	-
Boscalid	F	188425-85-6	0.0109	-	-
Cyprodinil	F	121552-61-2	0.0016	-	-
Epoxiconazole	F	133855-98-8	0.0158	-	-
Fenpropidine	F	67306-00-7	0.0064	-	-
Imazalil	F	35554-44-0	0.0082	-	-
Metrafenone	F	220899-03-6	0.0011	-	-
Picoxystrobin	F	117428-22-5	0.0013	-	-
Propiconazole	F	60207-90-1	0.0044	-	-
Prothioconazole	F	178928-70-6	0.0292	-	-
Pyraclostrobin	F	175013-18-0	0.0179	-	-
Tebuconazole	F	107534-96-3	0.0423	-	-
Thiabendazole	F	148-79-8	0.0001	-	-
Alpha-cypermethrin	I	67375-30-8	0.003	-	-

Cypermethrin	I	52315-07-8	0.0054	-	-
Dimethoate	I	60-51-5	0.0065	-	-
Gamma-cyhalothrin	I	76703-62-3	0.00001	-	-
Lambda-cyhalothrin	I	91465-08-6	0.0004	-	-
Pirimicarb	I	23103-98-2	0.0065	-	-
Tau-fluvalinate	I	102851-06-9	0.0029	-	-
Total (in a life cycle)			0.60	0.998	21.65

Assumptions:

[1] Data source: [±](Ørum and Samsøe-Petersen, 2014); [±±]after SEGES (2010) for the total life cycle years.

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