

Environmental Impact Assessment of wheat straw based Alkyl polyglucosides produced using novel chemical approaches

Supplementary information

1 Appendix

1.1 Life Cycle model Description

Conventionally, studies have opted for commercial life cycle assessment software including Gabi and Simapro. Though this approach offers reliability there are some limitations that can have an impact on the final outcome. Firstly, GaBi does not offer the flexibility for a custom-based system definition. SimaPro on the other hand has some key limitations. For example, the gross energy-use emissions of a product, which conventionally are sensitive to a region-specific sources of energy, must be precisely predicted. The source of electricity will have a very different impact on the environment. Regionally specific energy (e.g. energy mix, type of power-plants, conversion efficiencies) are not captured by the LCI database employed in SimaPro. In order to overcome these limitations, a devoted “cradle to gate” life cycle assessment model has been developed as a part of this study to project the environmental impact of a given product.

The LCA model developed for this study is composed of the following modules

<i>Biom_cult. ems.</i>	Biomass Cultivation
<i>LU_ems.</i>	Land use emissions
<i>Pre_Pro. ems.</i>	Pre-processing emissions
<i>Bio_ref. ems.</i>	Bio refining emissions
<i>Transp. ems.</i>	Biomass, feedstock and product transportation emissions
<i>LC_Env.I</i>	Life Cycle Environmental Impact
<i>LC_cost</i>	Life cycle costs
<i>LCI_EF and prices</i>	Life Cycle inventory: Emissions factors and Unit prices
<i>Soil N Chemistry</i>	Soils N ₂ O emissions
<i>LU standards</i>	Land use factors

Upon populating each of the module with appropriate input (material and energy) specifications, the eco-indicators (e.g. GHG_D and fossil-energy footprint) is calculated and summarily quantified in the “***LC_Env.I***” module. Figure A.1 presents the screenshot of the spreadsheet model developed to assess the life cycle environmental impact of the WS-APG and PW-APG in parallel.

Calculation of GHG_D emissions within the life cycle of WS-APG

a) Method for calculating life cycle emissions from material and energy consumption

GHG_D associated to materials consumed during this stage is empirically quantified using equation 1.1.1.

$$Stage_material_{GHG_D} = \sum_{i=1}^x M_{ini} \times EF_i \quad \text{Eq 1.1.1}$$

where,

M_{in} = Material input (kg or m³) and

EF = relevant emission factors (kgCO₂eq.kg⁻¹ or m³ of the material)

i-x = “1 to x” refers to the agricultural input which includes fertilizers, pesticides, seeds, water

GHG_D associated to materials consumed during this stage is empirically quantified using equation 1.1.2.

$$Stage_energy\ GHG = \sum_{i=1}^2 E_{ini} \times EF_i \quad \text{Eq 1.1.2}$$

where,

E_{in} = Quantified electricity consumed in a given life stage (kWh or l)

i= 1 - 2 = refer to electricity or fuel consumed

EF = Relevant (national average) emission factors (kgCO₂.kWh⁻¹ of the energy consumed)

GHG_D for irrigation water based on the amount of energy consumed and energy source used is calculated according to the equation in Eq 1.1.3a and Eq 1.1.3b. For water supply in Indonesia, use of coal based electricity was found to produce 0.99 gCO₂ eq.

$$E_{use_irr.water} (kWh) = \frac{9.8 (ms^{-2}) \times lift_{water} \times mass_{water}(kg)}{3.6 \times 10^6 \times \eta} \quad \text{Eq 1.1.3a}$$

where,

$E_{use_irr.water}$ = Energy consumed for irrigation (kWh)

$lift_{water}$ = ground water lifting distance (m), 1m assumed in this study

$mass_{water}$ = mass of water lifted (kg)

η = lift efficiency(%), 98% assumed for this study

$$Stage_water\ GHG = E_{use_irr.water} \times EF_i \quad \text{Eq 1.1.3b}$$

b) Calculation of direct GHG emissions attributable to transportation of commodities

$$Transp.GHG_D = \left[\frac{\sum_{i=1}^n payload_{1-n} \times distance_{1-n} \times EF_{veh.ems}}{Total\ mass\ of\ APG\ synthesised} \right] \times 10^3$$

Eq
1.1.4a

where,

$payload_{1-n}$ = Mass of the commodity transported between individual destinations
(tonnes)

$distance_{1-n}$ = distance between destinations (km)

$EF_{veh.ems}$ = vehicle-specific emission factor (kgCO₂eq tonne.km⁻¹)

[Note: 10³ used to convert tonnes to kg conversion]

$$Transp.GHG = Transp.(F - P)_{GHG} + Transp.(P - R)_{GHG} + Transp.(R - S.i)_{GHG}$$

Eq 1.1.4b

where,

$Transp.GHG$ = Total transportation emissions (kgCO₂eq.g⁻¹ APG)

$Transp.(F - P)_{GHG}$ = Emissions from transportation farm and pre-processing plant (kgCO₂eq.g⁻¹ AF

$Transp.(P - R)_{GHG}$ = Emissions from transportation pre-processing plant to refinery (kgCO₂eq.g⁻¹ AP

$Transp.(R - S.i)_{GHG}$ = Emissions from transportation Refinery gate to secondary industry (kgCO₂eq.g⁻¹ APG)

Appendix 1.2 : A flexible material and energy inventory developed for the model to undertake LCA for high value chemicals

Location	Materials (unit)	Sub-section	Emission factor (kg.CO2eq.unit ⁻¹)	Sources : Commodity Emission factor
UK	N-Fertiliser (general) (kg)	General	5.88	Defra, 2015
UK	N-Fertiliser (general) (kg)	Urea	3.31	Ecoinvent 2.2, 2010; Urea ammonium nitrate, as N, at regional storehouse (RER)
UK	N-Fertiliser (general) (kg)	Ammonium Nitrate	8.55	Ecoinvent 2.2, 2010; ammonium nitrate, as N, at regional storehouse (RER)
UK	N-Fertiliser (general) (kg)	Ammonium sulphate	2.69	Ecoinvent 2.2, 2010; Dataset : ammonium sulphate, as N, at regional storehouse (RER)
UK	N-Fertiliser (general) (kg)	Ammonium nitrate phosphate	5.27	Ecoinvent 2.2, 2010; Dataset : ammonium nitrate phosphate, as N, at regional storehouse (RER)
UK	N-Fertiliser (general) (kg)	Diammonium Phosphate	2.80	Ecoinvent 2.2, 2010; Dataset :Diammonium nitrate, as N, at regional storehouse (RER)
UK	N-Fertiliser (general) (kg)	Calcium ammonium nitrate	8.66	Ecoinvent 2.2, 2010; Dataset Calcium ammonium nitrate, as N, at regional storehouse (RER)
UK	N-Fertiliser (general) (kg)	N-Field Emissions (N2O)	4.87	Calculation of N2O emissions from N-fertiliser application according to IPCC methodology
EU	Other fertilisers (kg)	Triple super phosphate (TSP)	1.66	Ecoinvent 2.2, 2010; Dataset :Diammonium nitrate, as N, at regional storehouse (RER)
EU	Other fertilisers (kg)	Single super phosphate (SSP)	0.66	Ecoinvent 2.2, 2010; Dataset :Diammonium nitrate, as N, at regional storehouse (RER)
UK	Other fertilisers (kg)	P	0.71	Defra, 2015
EU	Other fertilisers (kg)	P2O5	1.01	Biograce. 2011
UK	Other fertilisers (kg)	K	0.47	Defra, 2015
EU	Other fertilisers (kg)	K2O	0.57	Biograce. 2012
EU	Other fertilisers (kg)	CaO	0.13	Biograce. 2013
EU	Other fertilisers (kg)	Magnesium oxide	1.06	Ecoinvent 2.2, 2010; Magnesium oxide, at plant (RER)
EU	Other fertilisers (kg)	Sulphate	0.58	Biograce. 2013
EU	Liming agents	Lime (CaCo3)	0.44	
EU	Liming agents	Dolomite (CaMg(CO2)2)	0.48	
EU	Liming agents	Calcium	0.785	

		ammonium nitrate (CAN)		
EU	Liming agents	Quicklime (CaO)		
EU	Pesticides (kg)	Aldrin	0.5	
EU	Pesticides (kg)	Chlodane	0.95	
EU	Pesticides (kg)	DDT	0.05	
EU	Pesticides (kg)	Dieldrin	0.15	
EU	Pesticides (kg)	Endrin	0.05	
EU	Pesticides (kg)	Heptachlor	0.95	
EU	Pesticides (kg)	Hexachlorobenzene	0.5	
EU	Pesticides (kg)	Mirex	0.15	
EU	Pesticides (kg)	Toxaphene	0.15	
EU	Pesticides (kg)	Pentachlorophenol	0.95	
UK	Pesticides (kg)	Metaldehyde (formulation 4%)	0.59	
EU	Pesticides (kg)	Lindane	0.5	
UK	Pesticides (kg)	Dimethoate & Chlorpyrifos	5.41	Defra, 2015
Indonesia	Pesticides (kg)	ParaQuat®	18.00	Guilbot et al, 2014
UK	Compost (kg)	Organic	0.02	Defra, 2015
UK	Irrigation water (m3)	Irrigation water	0.02	Defra, 2015
EU	Process (distilled/ deionised) water (m3)	Process water	0.00	Ecoinvent 2.2, 2010; tap water, at user (RER)
Indonesia	Seeds (individual)	Oil Palm	0.34	Halimah et al, 2013
EU	Seeds (kg)	Corn	1.93	
UK	Seeds (kg)	Rapeseed	0.61	Defra, 2015
EU	Seeds (kg)	Soybean	0.96	
EU	Seeds (kg)	Sugarbeat	3.54	Biograce, 2011
EU	Seeds (kg)	Sugarcane	0.00	Biograce, 2011
EU	Seeds (kg)	Rye	0.38	
EU	Seeds (kg)	Sunflower	0.73	Biograce, 2011
UK	Seeds (kg)	wheat	0.28	Defra, 2015
Indonesia	Electricity (kWh)	Local mix	0.85	Ecoinvent 2010

UK	Electricity (kWh)	UK Mix (average)	0.36	Defra, 2015
UK	Electricity (kWh)	CHP - Natural gas	0.00	Decc, 2015
UK	Electricity (kWh)	CHP-Waste gas	0.26	Decc, 2016
UK	Electricity (kWh)	CHP - Bio	0.00	Decc, 2017
v	Electricity (kWh)	Natural gas	0.18	
EU	Electricity (kWh)	Coal and lignite	0.37	
EU	Electricity (kWh)	Oil	0.23	
EU	Electricity (kWh)	Nuclear	0.00	
EU	Electricity (kWh)	Biorenewable	0.00	
EU	Electricity (kWh)	Biodiesel	0.00	
EU	Electricity (kWh)	Blast furnace gas	1.05	
EU	Electricity (kWh)	Domestic refuse	0.08	
EU	Electricity (kWh)	Ethane	0.18	
EU	Electricity (kWh)	Fuel Oil	0.27	
EU	Electricity (kWh)	Gas oil	0.27	
EU	Electricity (kWh)	Hydrogen	-	
EU	Electricity (kWh)	Methane	0.18	
EU	Electricity (kWh)	Mixed refinery gas	0.25	
EU	Electricity (kWh)	Waste Exhaust heat from high temperature process	0.03	
EU	Electricity (kWh)	Wood fuel (chips, pellets)	0.00	
Indonesia	Electricity (derivatives) (kg)	Steam	1.19	Calculated based on emissions factor for regional electricity mix from figures for average EU region
EU	Electricity (derivatives) (kg)	Steam	0.61	Ecoinvent 2.2, 2010
UK	HGV (diesel) (km)	HGV	0.12	Defra, 2015
UK	Fuel (l)	Diesel	2.68	
UK	Fuel (kg)	Oil		
UK	Fuel (l)	Diesel	2.68	Defra/DECC GHG Conversion Factors for Company Reporting (2011 update) and National Atmospheric Emissions Inventory (NAEI)
Indonesia	Fuel (l)	Diesel	2.68	
UK	Fuel (kg)	Petrol	3.14	

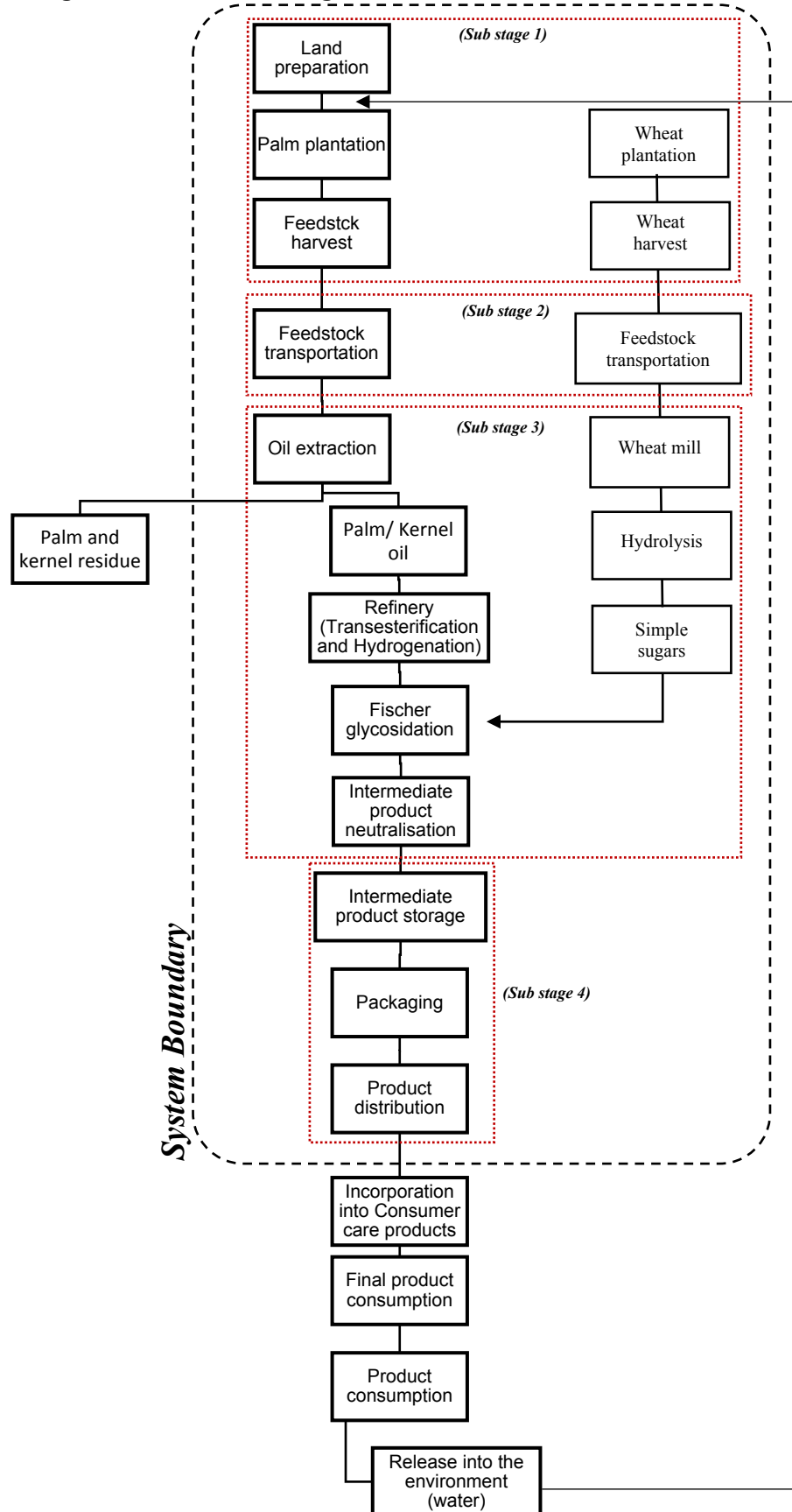
	Fuel (m3)	Natural Gas	7.15	
UK	Fuel (kg)	Coal and lignite	2.46	
Indonesia	Fuel (kg)	Coal	2.46	
Indonesia	Fuel (kg)	Marine fuel Oil	3.24	
UK	Fuel (kg)	Aviation kerosene	3.18	
UK	Air Cargo (Kerosene) (tonne.km)	Domestic	5.45	
UK	Air Cargo (Kerosene) (tonne.km)	Short Haul	2.31	
UK	Air Cargo (Kerosene) (tonne.km)	Long Haul	1.28	
UK	Air Cargo (Kerosene) (tonne.km)	International	1.28	
UK	Rail (tonne. km)	Rail	0.03	
UK	Sea tanker (tonne.km)	Crude tanker	0.06	
UK	Sea tanker (tonne.km)	Products tanker	0.09	
UK	Sea tanker (tonne.km)	Chemical tanker	0.09	
UK	Sea tanker (tonne.km)	LNG Tanker	0.05	
UK	Sea tanker (tonne.km)	LPG Tanker	0.05	
EU	Mineral Acids (kg)	hydrochloric acid	0.75	Biograce, 2011
EU	Mineral Acids (kg)	Nitric acid		
EU	Mineral Acids (kg)	phosphoric acid	3.01	
EU	Mineral Acids (kg)	Sulphuric acid	0.21	
EU	Mineral Acids (kg)	Acetic acid		
EU	Mineral Acids (kg)	Citric acid		
EU	Bio-derived solvent (kg)	Cyrene (UoY)	0.23	
EU	Organic solvent (kg)	Ehtyl acetate	0.231	
EU	Base chemicals (kg)	Sodium hydroxide	0.47	ISCC, 2015
EU	Base chemicals (kg)	Potassium hydroxide	0.00	
EU	Base chemicals (kg)	Sodium carbonate	1.19	
EU	Base chemicals (kg)	Fuller's earth	0.20	
	Catalyst (kg)	Copper-chromite		
EU	Alcohols (kg)	Methanol	1.25	

EU	Alcohols (kg)	Ethanol		
EU	Gases (kg)	Methane	0.03	IPCC, 2013
EU	Gases (kg)	Ammonia	2.66	Biograce, 2011
EU	Gases (kg)	Nitrogen	0.43	
EU	Gases (kg)	Nitrous Oxide (N ₂ O)	0.30	IPCC, 2013
EU	Gases (kg)	Carbon Monoxide	0.00	Robinson DL, 2011
EU	Gases (kg)	water vapour	0.00	IPCC, 2014
EU	Gases (kg)	Hydrogen	0.92	ISCC, 2015
EU	Gases (kg)	Carbon Di-oxide	1.00	IPCC, 2013
EU	Subcritical/ supercritical Solvents (kg)	Carbon di-oxide (NG)	8.83	Wang L, 2008, energy consumption to produce 1 kg of ScCO ₂ ; estimated
EU	Subcritical/ supercritical Solvents (kg)	Carbon di-oxide (coal)	15.02	
EU	Subcritical/ supercritical Solvents (kg)	water		
EU	Subcritical/ supercritical Solvents (kg)	Methane		
EU	Subcritical/ supercritical Solvents (kg)	Ethane		
EU	Subcritical/ supercritical Solvents (kg)	Propane		
EU	Subcritical/ supercritical Solvents (kg)	Methanol		
EU	Subcritical/ supercritical Solvents (kg)	Ethanol		
EU	Subcritical/ supercritical Solvents (kg)	Acetone		
UK	Packaging material (kg)	LDPE	2.16	Defra, 2015
UK	Packaging material (kg)	PET	2.16	
UK	Packaging material (kg)	PP	2.16	
UK	Packaging material (kg)	PS	2.16	
UK	Packaging material (kg)	PVC	2.16	
UK	Packaging material (kg)	HDPE	2.16	
UK	Paper and Board (kg)	Paper	0.68	
UK	Paper and Board (kg)	Board	0.68	
UK	Paper and Board (kg)	Mixed	0.68	

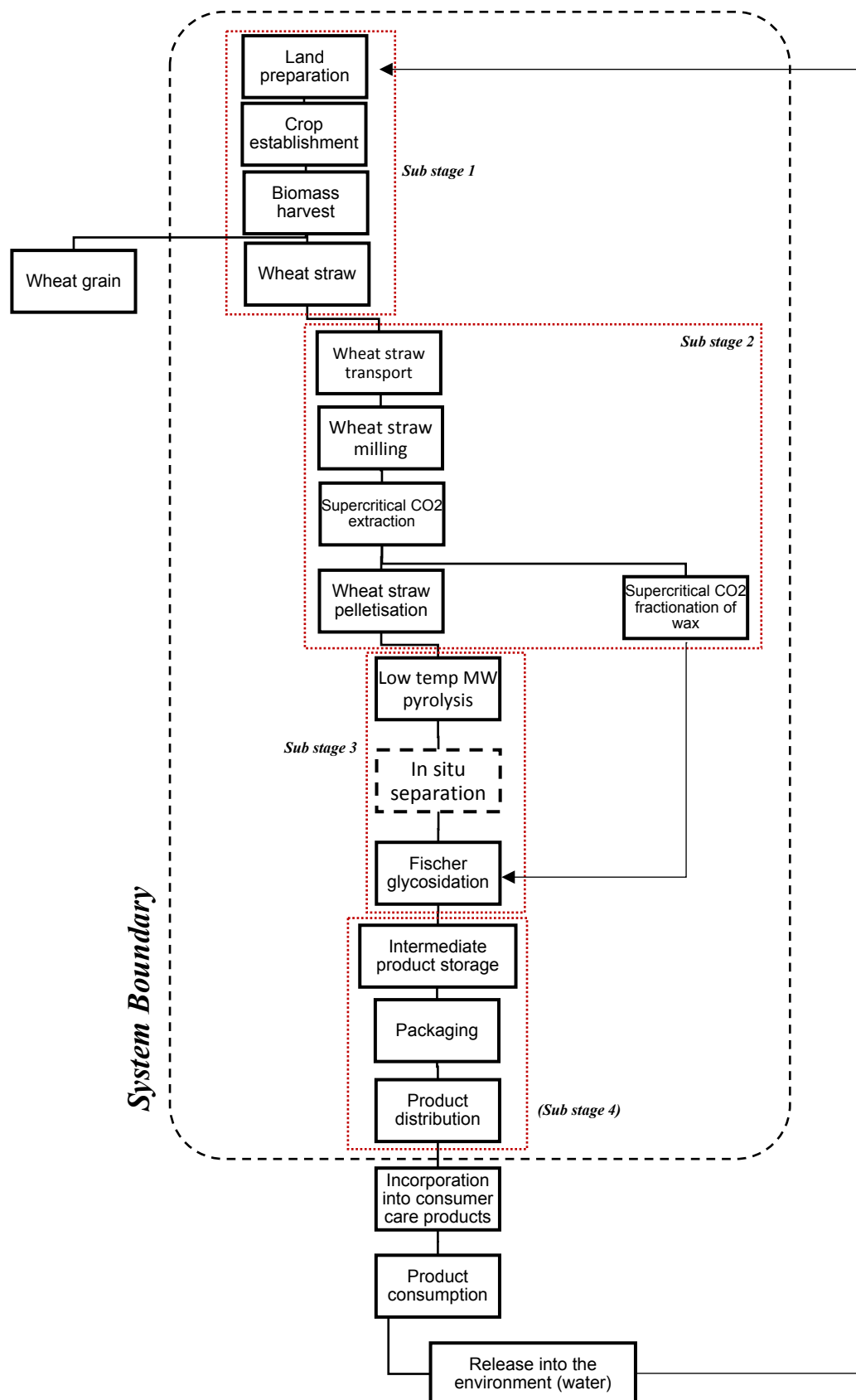
UK	Waste water Treatment (kg)		0.02	ISCC, 2015
Indonesia	Waste water Treatment (kg)		0.14	
Indonesia	Waste water treatment (kg)	POME treatment	0.18	
UK	Recycled by-products	Commercial and Industrial waste (Treated)	0.02	
Indonesia	Waste treatment (kg)	Empty Fruit bunch for mulch	0.03	
UK	Combustible	Biochar	-0.662	

1.3 Cradle-Grave life stages of Baseline and analysis pathway for APG production

APG production using Palm kernel and Wheat grain



APG production using Palm kernel and Wheat grain



Assumptions for LCA: Energy mix and associated data are regionally variable and, therefore, regional-specific data has been adopted here. Appropriate emissions factors (EFs) are used in both WS-APG and PW-APG processes where more specific data are lacking.

The complete chemical process for the synthesis of WS-APG were established prior to conducting the LCA. The cradle-grave life cycle stages of the analysis and baseline pathway are as follows [of which those italicised fall outside the scope of this analysis].

1. Raw material (biomass) acquisition – biomass procurement;
2. Biomass transportation - field to pre-processing plant;
3. Pre-processing phase – preparation of feedstock from biomass;
4. Feedstock transportation – pre-processing plant to refinery;
5. Refinery – for synthesis of bio-surfactants (intermediate, high-value chemicals);
6. Packaging and storage;
7. Product Distribution – transportation to local industries or whole-sale retailer;
8. Final Product synthesis – detergents, cosmetics or other personal care products;
9. Final product distribution;
10. *Product consumption;*
11. *Elements of products released and bio-degraded (in water or soil).*

1.4 Definition of Direct N₂O emissions

[**Note:** HGCA has adopted potential N₂O emissions predicted by Reay et al (2012) and the UK-DNDC model]. Based on analysis conducted at various sites across the UK, N₂O emissions from agricultural land are in the range of 1.6-4.36 kg of N₂O ha⁻¹. However, inclusion of emissions from wheat straw (residues) left on the field increased the emissions rates to 6.15kg of N₂O ha⁻¹ ⁵. This figure when simplified to N-fertilisers resulted in 0.0132 kgN₂O-N.kg⁻¹ of N fertiliser applied, while IPCC under-estimated N₂O emissions to be 0.0075 kg N₂O-N.kg⁻¹ of N-fertilisers added ¹. The unit ‘N₂O-N.kg⁻¹’ of N fertiliser corresponds to the emissions associated with the nitrogen component of the synthetic fertiliser/ compost. In addition to the synthetic N application, within our emissions inventory, N₂O emissions from organic compost applications to the field are also accounted. The nitrogen content of compost was assumed to be 0.6% based on finding of other studies based in the UK, ⁵⁻⁷ correcting the N₂O-N emissions to 0.0144 kgN₂O-N.kg⁻¹ of fertiliser, which was also suggested by HCGA ⁵ and Reay et al ⁷.

The method of converting N₂O- N to CO₂ equivalent emissions has been presented below

$$Field - N_2O_{GHG_D} = \left[Field N_2O \times \frac{N_2O_{Mm}}{N_{2Mm}} \right] \times GWP_{N_2O} \quad Eq 2$$

where

$$\begin{aligned} Field - N_2O_{GHG_D} &= CO_2 \text{ equivalent of Field } N_2O \text{ emissions (kgCO}_2\text{eq.ha}^{-1}) \\ Field N_2O &= Field N_2O\text{-N release (kgN}_2\text{O-N.ha}^{-1}) \\ N_2O_{Mm} &= \text{Molar mass of nitrous oxide} \\ N_{2Mm} &= \text{Molar mass of nitrogen} \\ GWP_{N_2O} &= \text{Global warming potential of agricultural } N_2O \text{ [i.e. } 298 \text{ kgCO}_2\text{eq.kg}^{-1} \text{ of N]}^1 \end{aligned}$$

¹ Source: IPCC, 2008]

1.5 Assumptions for Land Use Emissions estimation

- Land use emissions estimated using this method is restricted to a specific crop, grown in a specific soil type in a specific climatic region.
- This model adopts a metric of carbon equivalent of 1 kg of soil and vegetation to be 3.664 kg of CO₂ as suggested by the authors and also a conversion factor suggested by the IPCC, 2006^{3,4}.
- The two main factors that contribute to changes in the carbon stock of a given natural land are the climate type and soil type of the user-specified global region.
- In the default scenario, the period of cropland establishment was assumed to be more than 100 years as a result of which any emission from CO₂ emissions is assumed to have been neutralised via amortisation. Therefore, existing croplands do not inflict any LUE. However, in the case of baseline analysis, the authors of the baseline study have assumed land conversion from primary forests and grasslands to croplands. This scenario is likely to induce land use emissions based on the fraction of natural land types converted. The fraction of existing croplands, primary forests and grasslands converted for the establishment of oil palm plantations are 8%, 61% and 31% respectively.

Table 1 : SOC_{st} (Standard Soil Organic Carbon within 0- 30 cm of Top soil)

Climatic Regions	Standard Soil Organic Carbon (SOC _{st}) (0-30 cm of top soil)					
	HAC *	LAC*	Sandy soil	Spodic soil	Volcanic soil	Wetlands soil
Boreal	68	0	10	117	20	146
Cold Temperate, dry	50	33	34	0	20	87
Cold temperate, moist	95	85	71	115	130	87
Warm temperate, dry	38	24	19	0	70	88
Warm temperate moist	88	63	34	0	80	88
Tropical, dry	38	35	31	0	50	86
Tropical. Moist	65	47	39	0	70	86
Tropical, wet	44	60	66	0	130	86
Tropical, montane	88	63	34	0	80	86

Note:
Source: Official Journal of the European Union ; 2010; Commission Decision of 10 June 2010 on guidelines for the calculation of land carbon stocks for the purpose of Annex V to Directive 2009/28/EC
 * High Activity and Low Activity clay soils

The soil organic carbon stock of the original land is calculated using the *equations 6.1- 6.4*

$$SOC_A = SOC_{St} \times F_{lu} \times F_{mg} \times F_i \quad \text{Eq 1.1}$$

where,

= Soil Organic Carbon after stock change (land conversion) (tC.ha⁻¹yr⁻¹)

SOC_A

SOC_{St} = Standard Soil Organic Carbon in the first 0-30 cm of topsoil layer, (tC.ha⁻¹yr⁻¹)

F_{lu} = Land use factor

F_{mg} = Management factor

F_i = Carbon Input Intensity factor

The vegetation carbon stock (C_{veg}) for established plantation is to be predicted using the equation 6.2

$$C_{veg} = C_{Bm} + C_{DOM} \quad Eq\ 6.2$$

Where,

C_{veg} = above and below ground vegetation carbon stock, (tC.ha⁻¹yr⁻¹)

C_{Bm} = above and below ground carbon stock in living biomass, (tC.ha⁻¹ yr⁻¹)

C_{DOM} = above and below ground carbon stock in dead organic matter, (tC.ha⁻¹yr⁻¹)

The total carbon stock of the original land, CS_{actual} (soil + vegetation) is measured as tC.ha⁻¹.yr⁻¹, using equation 6.3

$$CS_{actual} = SOC_A + C_{veg} \quad Eq\ 6.3$$

Upon prediction of original land carbon stock (CS_{ref}) (as presented in equation 6.4), the soil (SOC_{ref}) and vegetation (C_{veg}) carbon stock of the reference crop per unit area is calculated from the default values provided in the guidelines in the reference literature³

$$CS_{ref} = SOC_{ref} + C_{ref.veg} \quad Eq\ 6.4$$

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