Supporting information

Table S.1 Crop rotation in the six fields over five years (2003-2007)

	2003	**2004**	**2005**	**2006**	**2007**
Field 1	Sugar beet	Winter Wheat	Set-aside	Winter wheat	oilseed rape
Field 2	Spring Barley	Spring Barley	Potatoes	Winter wheat	Sugar beet
Field 3	Spring Barley	Spring Barley	Sugar beet	Winter wheat	Oilseed rape
Field 4	Potatoes	Winter Wheat	Set-aside	Winter wheat	oilseed rape
Field 5	Sugar beet	Winter Barley	Potatoes	Winter wheat	Potatoes
Field 6	Potatoes	Winter Wheat	Sugar beet	Winter wheat	Spring Barley

Table S.2 Summary for the field operations during crop rotation (2003-2007)

Crop	Planting date	Harvesting date	Tillage date	Tillage methods
Sugar beet	28th April	17th Nov	15th March	Plough (20cm)
Spring barley	1st Mar	17th Aug	15th Feb 20th Feb	Plough (20cm) Power Harrowing (20cm)
Winter barley	15th Dec	17th Aug	20th Nov 10th Dec	Plough (20cm) Power Harrowing(20cm)
Potato	5th April	3rd Oct	20-Mar	Plough (30cm)
Oilseed rape	30th Aug	17th Aug	20th Aug 25th Aug	Plough (20cm) Power harrowing (20cm)
Winter wheat	30th Sep	17th Aug	15th Sep	Plough (20cm)

Table S.3 Fertilizer overall application rate[1] at Heygates Farm during crop rotation

Crop year 2003				
	Sugar beet	**Spring barley**	**Potato**	
Area %	26.98%	44.36%	28.66%	
N (t/ha)	1.27E-01	1.38E-01	1.71E-01	
P_2O_5 (t/ha)	3.63E-02	2.34E-02	1.29E-01	
K_2O (t/ha)	1.68E-01	4.68E-02	2.69E-01	
MgO (t/ha)	8.01E-02	5.77E-03	1.29E-02	
SO_3 (t/ha)	1.04E-02	7.41E-02	0.0	
Na_2O (t/ha)	2.60E-01	0.0	0.0	
Limestone (t/ha)	5.13E-03	4.06E-03	0.0	
Crop year 2004				
	Winter Wheat	**Spring barley**	**Winter barley**	
Area %	35.73%	44.36%	19.91%	
N (t/ha)	2.15E-01	1.18E-01	2.15E-01	
P_2O_5 (t/ha)	7.30E-03	2.34E-02	0.0	
K_2O (t/ha)	1.46E-02	4.67E-02	0.0	
MgO (t/ha)	1.80E-03	5.76E-03	0.0	
SO_3 (t/ha)	4.81E-02	5.61E-02	4.46E-02	
Na_2O (t/ha)	0.0	0.0	0.0	
Limestone (t/ha)	1.27E-03	4.05E-03	0.0	
Crop year 2005				
	Set-aside	**Potato**	**Sugar beet**	
Area %	23.25%	49.30%	27.45%	
N (t/ha)	0.0	2.07E-01	7.87E-02	
P_2O_5 (t/ha)	0.0	1.97E-01	4.93E-02	
K_2O (t/ha)	0.0	2.97E-01	6.95E-02	
MgO (t/ha)	0.0	6.73E-02	6.36E-02	
SO_3 (t/ha)	0.0	0.0	0.0	
Na_2O (t/ha)	0.0	0.0	2.00E-01	
Limestone (t/ha)	0.0	0.0	0.0	
Crop year 2006 Winter wheat				
Area %	**100%**			
N (t/ha)	208.55			
P_2O_5 (t/ha)	4.84			
K_2O (t/ha)	8.80			
MgO (t/ha)	2.20			
SO_3 (t/ha)	27.02			
Limestone (t/ha)	9.83			
Crop year 2007				
	Spring barley	**Oilseed rape**	**Sugar beet**	**Potato**
Area %	13.60%	35.10%	31.87%	19.44%
N (t/ha)	9.86E-02	2.24E-01	1.03E-01	2.74E-01
P_2O_5 (t/ha)	2.08E-02	3.68E-02	4.77E-02	8.98E-02
K_2O (t/ha)	3.78E-02	3.68E-02	9.46E-02	2.70E-01
MgO (t/ha)	8.56E-03	0.0	5.77E-02	3.48E-02
SO_3 (t/ha)	7.13E-02	8.93E-02	0.0	0.0
Na_2O (t/ha)	0.0	0.0	1.40E-01	0.0
Limestone (t/ha)	2.95E-03	4.40E-02	0.0	0.0

Note: *1. Overall application rate is "calculated as the total quantity of nutrient divided by the total extent of area (including any areas without application of the fertilizer)" [1]*

Table S.4 C-content for wheat grain

	Wheat flour	Wheat feed	Wheat grain
Proportion (% of harvested grain)	77.00%	23.00%	100.00%
Moisture content (%)	14.00%	12.77%	14.50%
Starch (% of dry basis)	88.95%	63.47%	83.09%
Protein(% of dry basis)[2]	11.05%	17.16%	12.45%
Oil (% of dry basis)	NI[1]	7.76%	1.78%
Fiber (% of dry basis)	NI[1]	7.72%	1.78%
Ash (% of dry basis)	NI[1]	3.90%	0.90%
C content (% of dry basis)	45.56%	47.09%	45.91%

Notes:

1. NI=No information.

2. In Heygates lab tests, total N was analyzed, then protein content was estimated from equation %Protein =% Nitrogen × NF. Where NF =Nitrogen Factor; $NF_{FLOUR}=5.75$; $NF_{FEED}=6.25$.

The theoretical C sequestration was calculated according to the lab-derived composition of the wheat flour and wheat feed produced from flour milling at Heygates Ltd. The C contained in wheat protein was estimated as 54.55% based on the formula $C_{16}H_{24}O_5N_4$ [2]. Composition of oil was derived from the Phyllis database (76% C content dry basis) [3]. C content in fiber was estimated on the basis of typical composition of wheat fiber presented by Knudsen [4] where the C component in each anhydrous sugar monomer was calculated from its formula and lignin was assumed to contain 60% C [3]. Overall CO_2 'sequestered' into the wheat grain was estimated as 1.47kg CO_2/kg fresh grain (moisture content 14.5%).

Table S.5 Data source

Unit processes	Data sources
WBF production	
Wheat farming	Heygates Ltd
Wheat flour milling	Heygates Ltd
WBF production	Greenlight Product Ltd
PVOH production	[5-7]
Transportation	Greenlight Product Ltd and feedstock suppliers
WBF case study	
Extruded HDPE and LDPE resin and expandable PS production	EU average data [8]
Transformation of LDPE and expandable PS into foam	EU average EPS transformation data [9]
Cardboard production	Box Factory EU average data [10]
Coolbox case study	Brunel University, Hydropac Ltd, Foam Engineers Ltd
Display board case study	Caledonian Industries Ltd and assumptions
Construction case studies	Cordek Ltd, Brunel University and assumptions
End-of-life	
PE/EPS 100% close-loop recycling	Ecoinvent database v 2.0, Nextek Ltd
PE/EPS 100% landfill	Ecoinvent database v 2.0
PE/EPS 100% incineration	Ecoinvent database (v 2.0) with electricity and thermal energy export
WBF home and industrial composting	Lab-determined WBF composition and meta-analysis derived composting model [11]
WBF landfill	Lab-determined WBF composition and meta-analysis derived landfill model [11]
WBF anaerobic digestion (AD)	A commercial AD plant in the UK, laboratory research on WBF biodegradability and energy recovery under AD [12]

Table S.6 Sensitive factors affecting DNDC-simulated emissions

Trace gas emission/leaching	Highly sensitive factors	References
N_2O	Soil clay content /texture	[13-15]
	Soil organic C	
	Annual temperature	
	Soil pH	
	Annual precipitation	
	Soil temperature	
	Soil nitrate	
	Fertilizer type	
	Water management	
N_2	Annual precipitation	[13]
	Soil pH	
	Annual temperature	
	Soil organic C	
CO_2	Soil organic C	[13, 16]
	Soil clay content /texture	
	Annual temperature	
	Crop rotation crop residue	
	Annual precipitation	
CH_4	Soil texture/clay content	[16, 17]
	Soil pH	
	N fertilizer application rate	
	Crop rotation	
NO_3^-	Initial organic carbon	[13, 18]

Table S.7 IPCC vs. DNDC

	IPCC Tier 1	DNDC
Approach classification	Empirical model	Process-based model
Application	National GHGs inventory	Site specific & national GHGs inventory
N_2O emission pathway	Direct emissions Indirect emissions (air decomposition & leaching)	Direct field emissions
Factors considered	1) Fertilizer input 2) Crop residue	1) Fertilizer type and input 2) Crop rotation 3) Daily climate 4) Soil property and texture 5) Farm management
Uncertainty	Large degree of uncertainty	Uncertainties caused by variability of input data
Simulated results (average of 6 fields) kg N_2O/kg fresh wheat grain	Direct N_2O 5.86 E-04 Total emissions 7.55 E-04	Direct N_2O 1.43E-04

Table S.8 Characterized 'cradle-factory-gate' GWP100 profiles for wheat flour and WBF products (kg CO_2 eq per unit product)

		Average	Filed 1	Filed 2	Filed 3	Filed 4	Filed 5	Filed 6
1kg Wheat flour	DNDC	-0.75	-0.89	-0.50	-0.96	-0.89	-0.54	-0.70
	IPCC-direct	-0.61	-0.76	-0.37	-0.83	-0.77	-0.40	-0.58
	IPCC-total	-0.56	-0.72	-0.32	-0.78	-0.73	-0.35	-0.52
WBF coolbox	DNDC	0.24	0.20	0.31	0.18	0.20	0.30	0.25
	IPCC-direct	0.28	0.24	0.35	0.22	0.24	0.34	0.29
	IPCC-total	0.29	0.25	0.37	0.23	0.25	0.36	0.31
WBF refractory lining former	DNDC	83.81	56.43	130.34	43.40	56.81	123.15	91.99
	IPCC-direct	108.61	80.59	155.22	67.44	79.47	148.75	116.09
	IPCC-total	118.06	89.30	165.00	77.05	87.68	158.80	125.93
WBF display board	DNDC	0.59	0.50	0.76	0.45	0.50	0.73	0.62
	IPCC-direct	0.68	0.58	0.85	0.54	0.58	0.82	0.71
	IPCC-total	0.72	0.61	0.88	0.57	0.61	0.86	0.74

Table S.9 Sensitivity analysis on N_2O modeling approaches.

Whole life cycle with diverse end-of-life						
	Display board HDPE			Refractory lining former virgin EPS		
	Landfill	Incineration	Recycling	Landfill	Incineration	Recycling
WBF AD scenario						
WBF-Average	green	green	yellow	green	green	purple
WBF-Field 1	green	green	green	green	green	purple
WBF-Field 2	green	green	purple	green	green	purple
WBF-Field 3	green	green	green	green	green	purple
WBF-Field 4	green	green	green	green	green	purple
WBF-Field 5	green	green	purple	green	green	purple
WBF-Field 6	green	green	yellow	green	green	purple
WBF landfill scenario						
WBF-Average	green	green	yellow	green	green	purple
WBF-Field 1	green	green	green	green	green	purple
WBF-Field 2	green	green	purple	green	green	purple
WBF-Field 3	green	green	green	green	green	purple
WBF-Field 4	green	green	green	green	green	purple
WBF-Field 5	green	green	purple	green	green	purple
WBF-Field 6	green	green	yellow	green	green	purple

Notes:

(green) *=WBFs with IPCC & DNDC model deliver lower GWP_{100} impact than petrochemical polymer*

(purple) *= WBFs with IPCC & DNDC model deliver higher GWP_{100} impact than petrochemical polymer*

(yellow) *= WBFs with DNDC model deliver lower GWP_{100} impact than petrochemical but with IPCC Tier 1 approach deliver higher GWP_{100} impact scores*

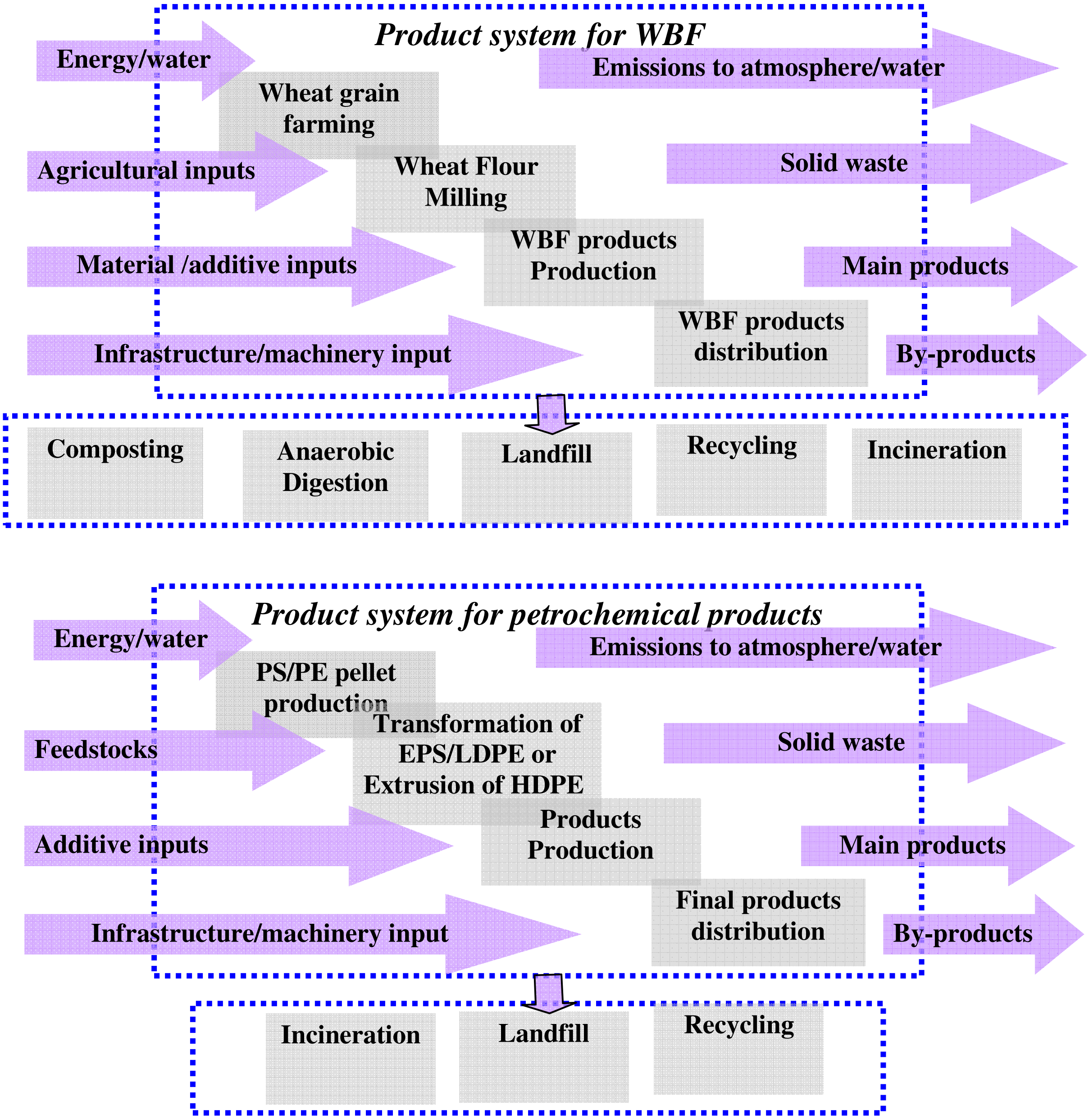

Figure S.1 Product system and system boundary for WBF and petrochemical products

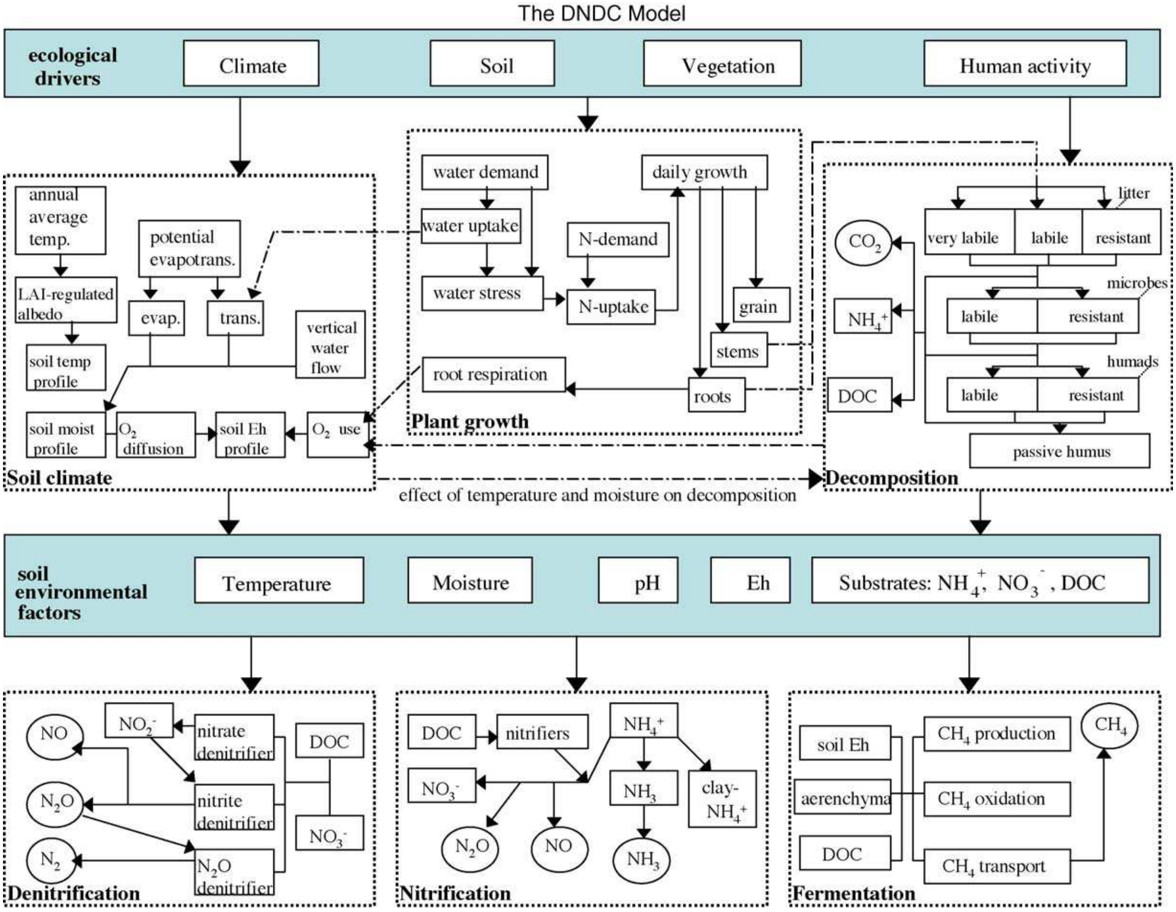

Figure S.2 Structure of DNDC model [18]

The DNDC model comprises two interacting components - the first comprises 3 sub-models (soil climate, plant growth and decomposition) and predicts soil environmental variables based on ecological drivers; the second component consists of nitrification, denitrification and fermentation sub-models simulating microbial activity and trace gas fluxes and N leaching.

The six sub-models play different parts and interact with each other. The soil climate sub-model integrates climate, soil properties and O_2 profile to simulate soil temperature and moisture [13, 19]. The climate, soil, crop parameters and field operations are integrated in the plant-growth sub-model to estimate crop growth, and its effects on soil temperature, moisture, available N and DOC etc. [20]. The decomposition sub-model mainly models 4 pools of soil organic carbon - microbial biomass, plant residues, active humus and passive humus; in addition, N dynamics during decomposition of organic matter in soil are simulated also (*e.g.* nitrogen mineralized enters the inorganic nitrogen pool as NH_4^+ which is either nitrified to NO^{3-} or is removed via crop-uptake, leaching or volatilization) [19, 21]. The denitrification sub-model is activated by increase in soil moisture or decrease in oxygen level from events like rainfall, flooding, and freezing temperatures (below -5°C) [21]; when these events occur, the production, consumption and diffusion of NO and N_2O are simulated. Another main source of NO and N_2O, nitrification, is included as a sub-model and the nitrification-induced NO and N_2O is calculated as a function of predicted nitrification rate and temperature and is influenced by the soil environmental variables. In addition, the NH_4^+/NH_3 equilibrium and functions for NH_3 production and volatilization are also included in the nitrification model [19]. The release of CH_4 is modelled in a fermentation sub-model, where CH_4 production, oxidation, and transport under submerged conditions is calculated based on fermentation equations [19].

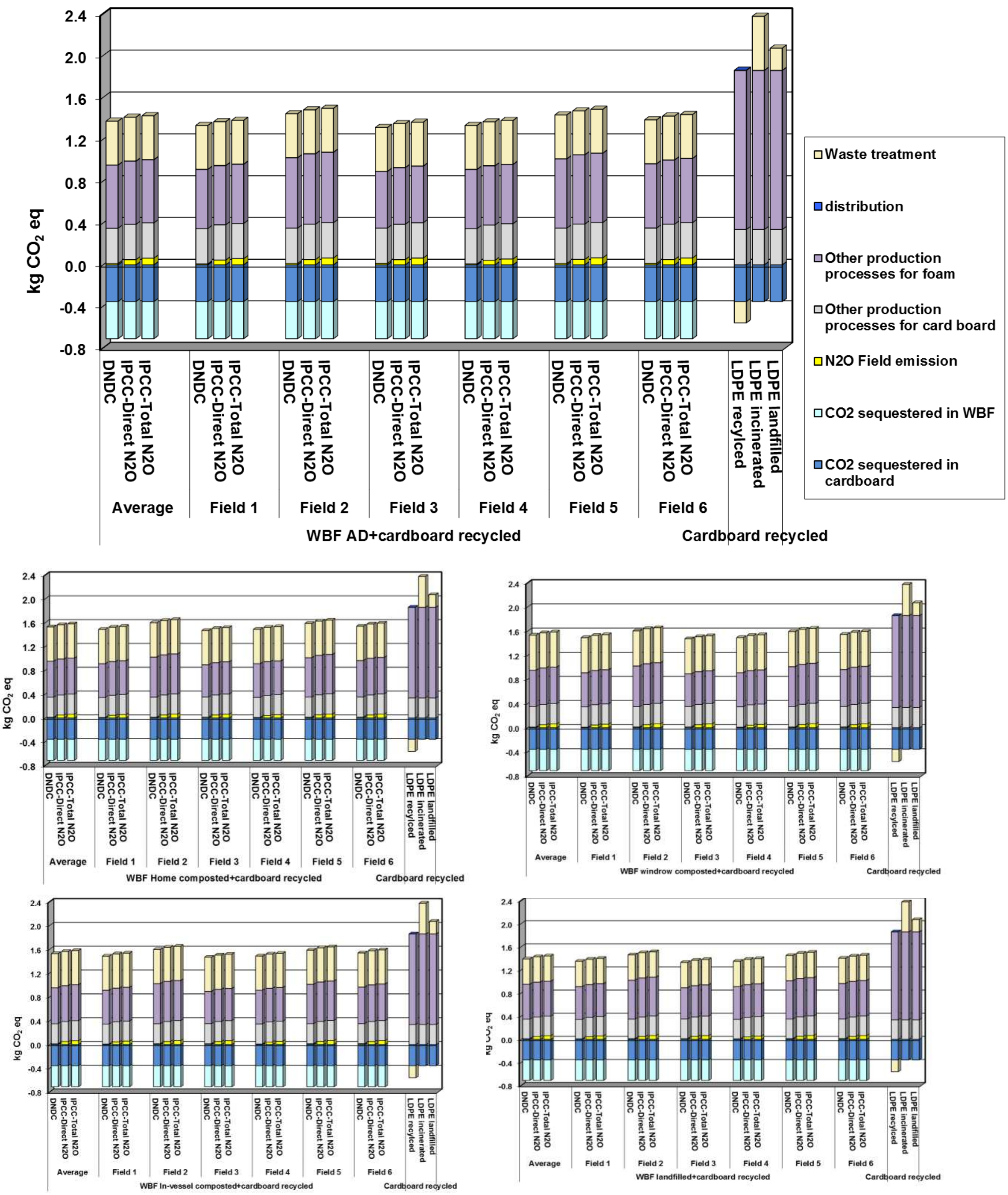

Figure S.3 Comparison of DNDC and IPCC modeling approach - characterized GWP_{100} profiles for life cycle of coolbox (unit: per coolbox)

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