Changes in greenhouse gas emissions due to the introduction of wheat straw ethanol in the context of European legislation: A consequential GHG assessment

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Abstract

Until today, first generation (1G) biofuels dominate the market for alternative fuels. The European Commission decided to cap 1G biofuels and promote second generation (2G) biofuels with the intention to reduce greenhouse gas (GHG) emissions, to limit the competition of food, feed and biofuels, as well as to improve societal approval. The assessment of consequences entailed to a shift from 1G to 2G biofuels is required to judge whether such a shift is advisable or not. According to the renewable energy directive (RED), GHG savings, need to be determined for all biofuels. By the end of 2020, fuel blends need to achieve a GHG reduction of 6%. Thus, GHG savings will determine the quantity of biofuel to be blended with fossil fuels and thereby eventually define the demand for biofuels. In this paper, the consequences of a shift from a 1G to a 2G biofuel is assessed by the example of bioethanol from wheat grains and straw. In total, three concepts of 2G ethanol production from wheat straw are considered: fermentation of C6-sugars with (1) co-production of feed, (2) coupled with biogas production and (3) co-fermentation of C5- and C6-sugars with co-production of feed. To determine the effect of the introduction of 2G ethanol, GHG savings according to RED are calculated first, and, in a second step, consequences of the shift from 1G to 2G ethanol are assessed by accounting for substitution mechanisms and emissions from direct and indirect land-use change (LUC). GHG savings of these 2G concepts according to RED methodology range from 103 to 105%. The shift from 1G ethanol to these 2G concepts is assessed by two scenarios: (1) additional production of 2G ethanol and (2) the replacement of 1G ethanol by 2G ethanol. Results indicate that GHG emissions decrease in scenario 1 if all surplus ethanol replaces fossil fuels. Under the given assumptions, the reduction in emissions ranges from 9.0 to 12.1 kg CO_2-eq. /GJ ethanol-gasoline blend. If 1G ethanol is replaced by 2G ethanol, GHG emission increase in a range from 7.5 to 16.5 kg CO_2-eq. /GJ fuel blend. This is mainly due to the provision of feed that needs to be supplied as a consequence of the shift in production: 1G ethanol production provides a high protein feed that needs to be provided by other means. Hence, the main driver for an increase in emissions is the provision of soybean meal and entailed emissions from LUC. A sensitivity analysis shows that these results are robust regarding input parameters and LUC assumptions. These findings point out that it is of utmost importance to assess changes induced by the introduction of novel fuels rather than assessing them isolated from market conditions. Based on these findings, it can be concluded that current and proposed legislation might trigger effects opposed to those intended.

Keywords

Straw ethanol, second generation biofuels (2G), GHG emissions, consequential LCA, Renewable Energy Directive

1. Introduction

As a consequence of the crude oil crises in 1973 and 1979/80, the production of liquid biofuels was expanded with the purpose of reducing the dependency on fossil fuels. In recent decades, the search for non-fossil alternatives has been propelled by the objective to reduce anthropogenic GHG emissions. Fuels based on vegetable oil, starch and sugar crops, named first generation (1G) biofuels, were the first biofuels that were brought to market maturity. Simultaneously, an increasing world population and changing consumption patterns have led to an increase in demand for agricultural commodities. As a consequence, second generation (2G) biofuels obtained from organic residues and wastes were strongly promoted as an alternative to 1G biofuels. The European Commission decided to cap the use of 1G biofuels to promote their phasing out [1,2]. In order to facilitate a reduction in GHG emissions, the European Commission decided that biofuel-fossil fuel blends are required to achieve a reduction in GHG emissions of 6% by 2020 [3]. The quantity of a biofuel to be blended with fossil fuel to achieve this target is determined by the GHG savings that are estimated through a calculation method defined in the RED [4]. As of 2017, only Germany has adopted this mechanism, while other countries still rely on fixed blending rates [5]. However, in the future, other European countries will transpose this mechanism into national legislation. At the moment, the European Commission is revising the RED for the period of 2021-2030 and the current draft indicates that a reduction in the share of 1G biofuels is envisaged [2]. In contrast, minimum targets of 2G biofuels are implemented and a trajectory is defined to facilitate an increase of the share of 2G/advanced biofuels. The predicted decrease in the energy demand of the transport sector by 7% from 2015 to 2030 should therefore result in a replacement of 1G biofuels with its 2G counterpart [6]. Among 2G biofuels, straw-based bioethanol presents one of the most promising concepts [7].

In this context, the present paper assesses the transition 1G to 2G biofuels, using the example of bioethanol production from wheat grains and straw cultivated in Germany. Thereby, the implications of the blending regulation based on GHG savings, as well as the proposed transition from 1G to 2G bioethanol, are discussed.

2. Literature overview and motivation

Recent political decisions have been accompanied by the interest to evaluate the environmental impacts of 1G and 2G biofuels (among other means of providing energy for transportation). In recent years, numerous studies addressed the environmental impacts of 2G biofuels by life cycle assessment (LCA). The reviews of Gerbrandt et al. [8], Morales et al. [9] and Borrion et al. [10], analyzing studies on bioethanol production from lignocellulosic feedstock covering for the time period from 1999 to 2015, indicate a reduction in GHG emissions due to the use of 2G bioethanol in comparison to fossil fuel. The studies comprised in these reviews show a high variation of important parameters such as the quantity of fertilizer that is applied, N_2O emissions resulting thereof, as well as ethanol and co-product (mainly electricity) yields [8–10]. Furthermore, the application of different LCA methodologies leads to complication when comparing various studies. The handling of arising co-products, the selection of a reference system and the functional unit have the highest impacts on results among methodological aspects. The chosen methodology usually depends on the type of analysis that is conducted: On the one hand, an attributional LCA (aLCA) seeks to analyze the environmental impacts of a specific product system or service and to provide an evaluation of environmental implications of different stages of the life cycle of a product [11]. The analyzed system is limited to the assessed product system. On the other hand, a consequential LCA (cLCA) seeks to assess changes in environmental impacts as a consequence of a change in a product system or as a result of a specific decision [11,12]. In this case, the analyzed system is expanded and accounts for market effects and other consequences that might occur.

In recent years, the focus has shifted to the use of LCA as a means to support (political) decision making [13]. This trend, reflected in the increased interest in cLCA studies, has been a driver and a consequence of the discussion on (indirect) land-use change (iLUC) triggered by biofuel demand. A vital debate evolved that revolves around the key question: which method is best to support robust (political) decision making? Due to its ability to reflect potential consequences of certain decisions, cLCA is considered by some to be a useful method to support policy making, cf. [14,15]. However, the fact that cLCA cannot accurately account for all market effects, that its results and hypotheses cannot be confirmed or falsified, and that emission reductions predicted by cLCAs do not result in emission reductions if not accompanied by appropriate political measures, has led to criticism [16,17]. In practice, the distinction between these two models is not that clear and a constructive dialogue leading to modeling frameworks that allow better support of decision making is needed [18].

This debate reflects the need of investigations that discuss both approaches in the context of political decision making. Recent studies on novel fuel production concepts applying aLCA or the RED methodology, mainly presenting a aLCA approach, report a reduction in GHG emissions in comparison to fossil reference systems [19–23]. However, the omission or inconsistent inclusion of substitution effects and other consequences on connected markets inhibits the drawing of a conclusion as to whether an introduction of the analyzed fuel is likely to result in a reduction in GHG emissions. The aLCAs of straw-based fuel and energy production conducted by Whittaker et al. [21] and Weiser et al. [23] present detailed discussions of methodological aspects regarding straw removal. In both cases, authors concluded that changes in energy and agricultural markets need to be addressed by means of cLCA to improve the understanding of consequences entailed to the analyzed system. Monteleone et al. [24] provide such a cLCA of straw-based electricity production in Southern Italy. A comparison of two conventional (agro-ecological and energetic valorization of straw) and one "innovative" concept (no-tillage practice, crop rotation) yields that the latter is the most preferable in terms of GHG emissions and the reduction of fossil energy demand. Lopes de Carvalho [25] assessed environmental impacts of the production of bioethanol in Brazil and its effect on the Brazilian economy and show that positive effects induced by 1G and 2G ethanol production can be counterbalanced by negative effects occurring elsewhere in the economy. Hamelin et al. [26] assessed the consequences of the production of biogas in Denmark and found a reduction in GHG emissions due to a shift from a fossil reference system to the production of biogas. Tonini et al. [27] conducted a detailed cLCA of bioelectricity, biomethane and bioethanol from 24 substrates produced in Northern Europe. The assessment of 1G and 2G substrates considers emissions from feedstock provision to the final use of the energy carrier in case of biofuels. The results indicate that only ethanol from household wastes and agricultural residues reduce GHG emissions. The substitution of fossil gasoline and 1G ethanol produced in Brazil has been assessed. In the latter case, emission reductions and increases, in case of 2G and 1G bioethanol respectively, are less pronounced. Bos et al. [28] conducted a cLCA of the coupled production of biodiesel, biopolyol and bioresin. This assessment is one of very few examples in which other co-products than energy or feed are considered. The assessment neglects the use of fuels and LUC effects. All products result in a decrease in emissions when fossil counterparts of co-products are replaced. Another cLCA of biodiesel from oil palm, soy and rapeseed by Corré et al. [29] showed GHG emissions ranging from 22 to 56 g CO_2-eq./ MJ biodiesel without considering LUC emissions. Escobar et al. [30] compared biodiesel from soy cultivated in Brazil with biodiesel from used cooking oil and found that the 2G fuel resulted in an emission reduction in contrast to soy-derived biodiesel. The main contributor is LUC in both cases. The cultivation of soy results in LUC emissions, whereas the production of biodiesel from used cooking oil reduces the demand of vegetable oil resulting in avoided LUC emissions. The assessment of iLUC emissions as a consequence of an increase in biofuel demand in Spain conducted by Garraín et al. [31] reveals iLUC emissions ranging from 16 to 56 g CO_2-eq./ MJ for bioethanol and from 22 to 52 g CO_2-eq./ MJ for biodiesel. Triggered iLUC effects are highly dependent on feedstock and the assumed substitutes. Therefore, the authors concluded that generic iLUC factors, as proposed by the European Commission, do not reflect these high variations. All these studies present assessments of consequences related to the provision of (co-)products of the analyzed biofuel system. However, due to the limitation of system boundaries excluding the production or use of fuel [19,27,28,30,31], the omission of LUC emissions [19,25,28,29] or inconsistent handling of co-products (e.g. mixture of aLCA and cLCA, as required by the RED) [19,22], most results do not allow to draw conclusions as to whether the use of a specific fuel is advisable in terms of GHG emissions or not. Furthermore, only one of these studies accounts for the implications on existing biofuel markets ([27]), while none considers the fuel-blending mechanism implemented by the European Commission.

In contrast to the available studies, the current work assesses the introduction of novel fuel concepts in the context of current legislative practice and envisaged political targets by analyzing a shift from an existing conventional 1G ethanol production from wheat grain to 2G ethanol from wheat straw. The current assessment comprises of market-driven effects entailed to the provision of co-products as well as consequences of current blending legislation that needs be transposed by European member states. This paper addresses these aspects which have not been addressed elsewhere and discusses them based on aLCA and cLCA methodology, thereby contributing to the ongoing debate concerning the capability of LCA to support political decision making. The following questions are answered using the example of 1G and 2G ethanol production in Germany:

(1) What are the emission hot-spots of producing bioethanol from wheat grain and wheat straw?
(2) How do the assessed concepts perform in regard to current legislative practice?
(3) What are possible consequences in GHG emissions of a shift from 1G to 2G bioethanol (envisaged by political measures) if potential market mechanisms are included?
(4) Is an assessment based on current legislative practice capable of reflecting these consequences?
(5) Will proposed legislation facilitate an overall reduction in GHG emissions?

In the light of the current revision of the RED, as well as the envisaged reduction of 1G biofuels and increase of 2G biofuels, the answers to these questions will provide detailed insights into possible implications of current political-decisions that will eventually shape the European and global biofuel industry for the upcoming decades.

3. Methodology

A two-step approach is followed to assess potential consequences of the introduction of 2G bioethanol from wheat straw:

- In a first step, GHG savings[1] are estimated based on the methodology laid down by RED. These GHG savings of any biofuel produced in a facility in operation before 1 January 2017 must amount to at least 50%. According to the RED methodology, emissions are allocated to all co-products, except for electricity for which a credit is given. Thereby, the RED methodology represents a mostly aLCA approach that disregards changes in emissions that occur due to the provision of co-products or due to other market driven effects that result from the introduction of a specific fuel.
- In a second step, emission changes resulting from the introduction of 2G ethanol are estimated by applying a consequential model that considers changes in blending

[1] The terminology „GHG savings", here and hereafter, exclusively refers to the value calculated by RED methodology (Eq. (1)). The terminology "GHG reduction" refers to the political target of reducting emissions compared to a fossil fuel comparator by 6% in 2020. Both cases do not present a change in emissions, as the applied RED methodology is not able to reflect these. In contrast, terms like "decrease" or "increase in GHG emission" refer to estimations of changes in emissions based on the consequential approach, thus respecting occurring changes in emission due to changes induced by the change in the (product) system, i.e. the introduction of 2G biofuel.

quantities (based on the RED methodology), occurring substitution mechanisms, market effects, LUC etc. As of the end of 2020, the final biofuel-fossil fuel blend must achieve a GHG reduction of 6 % [1]. Thus, the quantity of biofuel to be blended with a fossil fuel is defined by GHG savings determined by the RED methodology.

The calculation of GHG intensities was conducted with openLCA 1.4.2. Global warming potentials, as defined by the RED [4] and the Intergovernmental Panel on Climate Change [32], were applied for the determination of GHG savings according to RED methodology and for the consequential approach, respectively (Table S.1).

3.1 RED methodology

Regardless of the type of biofuel, its provision and use is regulated by the RED [1,4] and the fuel quality directive [3]. The RED, representing the most important political instrument, defines sustainability criteria for biofuel provision. Aside from GHG emissions, sustainability aspects, such as biodiversity and direct land-use change, are also addressed. Additionally, the RED defines a methodology to quantify GHG emission savings from the use and provision of biofuels. As of the end of 2020, the quantity of biofuels to be blended with fossil fuels is dependent on the achieved GHG emission savings based on the RED methodology (Eq. (1)):

$$GHG\ savings = \frac{GHG_f - GHG_b}{GHG_f} \quad (1)$$

where GHG_f represents the fossil fuel comparator of 83.8 g CO_2-eq./ MJ reflecting GHG emissions of fossil fuel provision and combustion and GHG_b presents the GHG emissions related to the provision of the biofuel [3]. Emissions originating from the combustion of biofuels are considered to be carbon neutral due to the biogenic origin of carbon. Emission reduction per MJ of fuel blend must amount to at least 6% compared to the fossil baseline comparator of 94.1 g CO_2-eq./MJ [1,33]. According to the legislation, both comparators are not fuel-specific and thus do not distinguish between diesel and gasoline. They are applied for all liquid fuels.

GHG emissions of biofuel provision comprise of: emissions from feedstock cultivation, the provision of energy and auxiliary materials, transport of materials and fuel distribution. In the case of several co-products of a product system, emissions and input are apportioned to all products.

- Inputs and outputs are allocated to products based on their lower heating value (LHV).
- Credits are given for feeding excess electricity into the grid, except when the used fuel is a co-product other than an agricultural residue. The credit equals the emissions caused by generating the respective amount of electricity using the same energy carrier.
- Credits are also provided for capturing biogenic CO_2 that replaces fossil-derived CO_2 used in commercial products and services.
- Electricity from biomass that is a co-product of the production process is treated as a co-product.

Allocation is accomplished in the following manner: Let P_i denote the quantity of product of process i that is needed to deliver the functional unit, I_i denote the total impact of process i per output of P_i, and α_i the allocation factor of P_i in process i with a total number of N processes, it follows that I_{FU}, the total impact per functional unit, can be expressed by equation (2).

$$I_{FU} = \sum_{i=1}^{N} \alpha_i\, P_i\, I_i \quad (2)$$

The allocation factor α of product P_u of a process delivering M products is determined by equation (3).

$$\alpha_u = \frac{\varepsilon_u\, P_u}{\sum_{u=1}^{M}(\varepsilon_u\, P_u)} \quad (3)$$

Where ε_u denotes the parameter on which the allocation is based on, i.e. LHV.

3.2 Consequential approach

A consequential life cycle assessment (LCA) reflects changes induced by marginal changes in the assessed production system or market [34]. Occurring changes due to displacement mechanisms are accounted for by estimating potential emission changes as a consequence of changes in demand of (co-)products and the respective reference products as well as induced emissions from LUC effects. Substitution mechanisms and LUC emissions are case-specific and will thus be explained in Table 3 and Table 4 subsequent to the description of scenarios, case-specific co-products and related substitution mechanisms described in section 4.2.1 to 4.2.3. Occurring LUC is estimated with a deterministic model through identification of marginal suppliers under consideration of legislative frameworks, trade statistics, market environments and past developments.

3.2.1 Feed as a co-product

The provision of feed as a co-product substitutes other feed products. In case of protein feed, a linear equation system is used to reflect the substitution of protein and feed energy. The replacement ratio is calculated with equations (7) and (8) [35].

$$nXP_{co-product} = \lambda\, nXP_{protein\,feed} + \mu\, nXP_{cereal} \quad (7)$$

$$ME_{co-product} = \lambda\, ME_{protein\,feed} + \mu\, ME_{cereal} \quad (8)$$

Where nXP, ME, λ and μ denote the digestible protein content, the metabolizable energy for cattle and the displacement ratios, respectively [35]. The production of meal for animal consumption is coupled with the production of vegetable oil [36–39]. When feed co-products reduce the demand for seed meal, resulting in a decrease in supply of meal that is substituted, seed oil production is reduced as well. In this case, oil will be supplied by another marginal supplier. By providing the respective quantity of oil to the market, meal will be supplied as well. The corresponding feedback loop and mathematical description of it is explained in the section 1.1 of the supplementary material.

3.2.2 Land-use change

The change of land-use results in changes in soil organic carbon (SOC) and above-ground vegetation. The respective changes in GHG emissions are estimated based on equations (9) and (10) [40,41].

$$\Delta C_{mineral} = \frac{(SOC_0 + C_{veg_0}) - (SOC_{0-T} + C_{veg_{0-T}})}{D} \quad (9)$$

$$SOC = \sum_{c,s,i}(SOC_{REF_{c,s,i}}\, F_{LU_{c,s,i}}\, F_{MG_{c,s,i}}\, F_{I_{c,s,i}}\, A_{c,s,i}) \quad (10)$$

Where: $\Delta C_{mineral}$ denotes the annual change of carbon (C) stocks in mineral soils and in above-ground biomass, SOC_0 the soil organic C stock in the last year of an inventory time period SOC_{0-T} soil organic C at the beginning of the inventory time period, C_{veg_0} and $C_{veg_{0-T}}$ the carbon stocks in above-ground biomass in the last year and the beginning of the inventory period, T the number of years over a single inventory time period in years, c the climate zone, s the soil type, i the set of management systems, SOC_{REF} the reference carbon stock, F_{LU} the stock change factor for the respective land-use systems, F_{MG} the stock change factor for the management regime, F_I the stock change factor for the input of organic matter, and A the assessed area. A time period, D, of 20 years is chosen.

4. System description

The production of 1G cereal grain ethanol and 2G wheat straw ethanol is assessed by hypothetical production facilities with a capacity of 150,000 m³ ethanol per year, i.e. facilities of medium production capacity. This capacity is chosen in order to reflect theoretical 2G ethanol facilities at the early stages of market maturity. Feedstock cultivation and fuel production is assumed to take place in Germany.

4.1 GHG savings according to RED methodology

Ethanol production comprises feedstock provision, feedstock conversion, fuel distribution, transport activities as well as the provision of energy and auxiliary materials. The reference year is 2020.

4.1.1 Wheat cultivation

Conventional wheat cultivation in Germany is assumed. Between 2005 and 2014, the yield of wheat fluctuated between 6.9 and 8.6 t/ha [42]. A slight positive trend in yields can be observed. In the present study a yield of 7.9 t/(ha a) is assumed [43]. The dry matter content (DM) of grains and straw ranges from 83 to 94% [44]. DM contents of 86% and 90% are assumed for grains and straw, respectively [43,45,46]. Fertilizer is applied according to nutrient extraction. Without straw removal, 118.9 kg ammonium nitrate-N, 25.1 kg phosphate-P, 34.0 kg K_2O-K and 8.2 kg Mg are applied per hectare and year. Nitrous oxide emissions from fertilizer application are estimated by the IPCC Tier 1 method [47]. Ammonia-N emissions are assumed to be 2.5% of applied N [48]. Nitrate emissions are estimated based on fertilizer input, soil and plant characteristics as well as annual precipitation [49].

The quantity of straw that can be harvested is based on the sustainable straw potential in Germany, assuming soils in good condition and adequate supply of N [23,50]. The assumed grain/straw ratio is 0.8 [23]. The calculated sustainable straw potential is 44.7% available straw (see section 2.1 of the supplementary material). The N, P, K, Mg and S content of straw is 0.55, 0.13, 1.45, 0.12 and 0.23% of fresh matter, respectively [51]. In case of straw removal, these nutrients are supplied by mineral fertilizer.

Grains are transported 120 km by truck [52]. The design of straw handling depends on straw requirements of the respective 2G ethanol facility. Straw is transported 3.6, 3.6 and 2.9 km by tractor to the intermediate storage and 93, 93 and 76 km by truck to the ethanol production facility in case of concept I, II and III, respectively (concepts are explained in section 4.1.3, straw handling and the estimation of transport distances are described in section 2.2 of the supplementary material).

4.1.2 Ethanol production from wheat grains

Preceding starch hydrolysis and transformation to sugars by the aid of enzymes, wheat grains are dry milled. Resulting sugars are fermented to yield ethanol. The purification of ethanol is accomplished by distillation / rectification. Finally, ethanol is dehydrated to a purity of 99.7% by molecular sieves. Aside from ethanol, the overall process yields wheat dust, fusel oils and stillage. The stillage is dried to a DM content of 90% to yield dried distiller's grains with solubles (DDGS), a high protein feed. The applied data are from operating facilities (Table 1). Emissions related to the provision of auxiliary materials and energy provision are based on ecoinvent v.3.2 data [53]. Energy is supplied by a natural gas boiler with a steam turbine; the electric and thermal efficiencies are 12.5 and 72.5%, respectively. Emissions of volatile organic compounds are estimated based on measurements [54]. CO_2 originating from the fermentation process is captured. This intercooled 5-stage compression process requires 0.43 MJ electricity/ kg CO_2 [55]. Finally, ethanol is transported 150 km by truck from the production facility to the depot and another 150 km to the filling station [56].

Table 1 Inventory data for 1G ethanol production from wheat grains.

Input	**Unit**	**Value**	**Reference**	**Output**	**Unit**	**Value**	**Reference**
Wheat grains	kg	3.39	[52,57]	Ethanol, 99.7%	kg	1	
Heat	MJ	10.80	[52,57]	DDGS, 90% DM	kg	1.08	[52,57]
Electricity	kWh	0.47	[52,55,57]	Electricity	kWh	0.05	
Sulfuric acid	kg	0.02	[52,57]	Fusel oils	kg	0.004	[52,57]
Sodium hydroxide	kg	0.02	[52,57]	Wastewater	L	4.82	[52,57]
Ammonia	kg	0.002	[52,57]				
Enzymes	kg	0.003	[52,57]	Emissions			
				Acetic Acid	kg	5.05E-05	Estimation based on [54]
				Ethanol	kg	1.52E-04	
				Ethyl Acetate	kg	1.85E-04	
				Lactic Acid	kg	2.70E-05	
				2-Furaldehyde	kg	3.37E-06	
				Acetaldehyde	kg	2.19E-04	
				Acrolein	kg	3.37E-06	
				Formaldehyde	kg	3.37E-06	
				Methanol	kg	3.37E-06	

4.1.3 Ethanol production from wheat straw

Three concepts of ethanol production from wheat straw are assessed (Figure 1).

I. C6 fermentation and co-production of feed
   - fermentation of C6-sugars to yield ethanol
   - thickening of C5-sugars to produces C5-molasses (DM 60%), a feed product

II. C6 fermentation and biogas production
   - fermentation of C6-sugars to yield ethanol
   - production of biogas from C5-sugars
   - purification and upgrading of biogas to natural gas quality
   - production of fertilizer products from digestate

III. Co-fermentation of C5- and C6-sugars with co-production of feed
   - co-fermentation of C5- and C6-sugars
   - thickening of residues, which can be sold as a feed product (DM 60%)

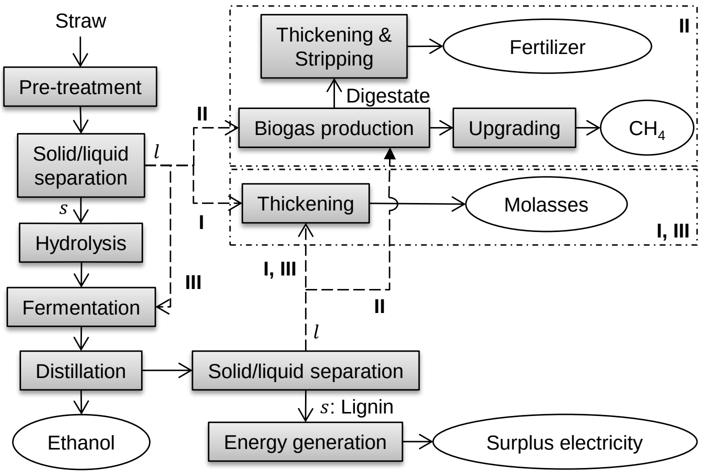

Figure 1 Assessed production concepts for the production of ethanol from wheat straw (bold roman numbers indicate process steps that belong to a specific concept; l – liquid phase, s – solid phase)

Dry wheat straw consists of 39.2% cellulose, 24.8% xylose, 22.4% Klason lignin, 2.7% arabinose, and 2% other sugars [46]. The moisture content before pre-treatment is 10%. The wheat straw is pre-treated by steam explosion, yielding a liquid phase rich in C5-sugars, e.g. xylose, arabinose and a solid stream rich in lignin and C6-sugars, e.g. glucose. Steam explosion is conducted at 190 °C for 10 minutes. The conversion efficiencies and the composition of wheat straw are listed in Table S.2. This setup is chosen due to its low yield of inhibiting compounds [58]. The following hydrolysis requires 20 mg enzymes/ g of cellulose [59]. The yields of glucose, xylose, arabinose and galactose are assumed to be 86, 68, 94 and 100%, respectively [58,60]. The ethanol yield from glucose, xylose and arabinose are 98, 93 and 54 %, respectively [52,61]. Ethanol fermentation requires 3 g enzymes/ t ethanol [52].

In all concepts, stillage is separated after fermentation into a liquid phase containing dissolved unfermented sugars and a solid stream mainly consisting of lignin and unfermented solid sugars. The solids are used to provide process heat and electricity. Emissions for energy generation from lignin are taken from the probas data base [62]. The efficiency of energy generation is optimized to provide heat and electricity according to process demands. Surplus electricity, if available, is a co-product. In all cases, CO_2 is captured as in case of 1G production.

In concepts I and III, the liquid stream is thickened to a DM of 60% to provide a feed product. It is assumed that 50% of the process water can be recycled. The remaining water is treated in a waste water treatment facility. In concept II, stillage containing 8 g volatile solids/ kg is used to produce biogas with a CH_4 content of 50% [63–65]. It is assumed that no additional heat is required as stillage contains latent heat when leaving the ethanol production process. Gas leakage of biogas production is assumed to be 1% [66,67]. Biogas is de-sulfurized by activated carbon before being purified by pressure swing adsorption; this cleaning process requires 2.1 10^{-4} kg activated carbon and 1.5 10^{-4} kg lubricant oil per m^3 purified gas [68]. Waste gas is flared and all emissions are accounted for as well. The methane slip (unburnt methane) that leaves the waste gas flare is 0.2% of the waste gas stream [69]. Bio-CH_4 is compressed and the energy content is adjusted to meet grid requirements by adding propane (0.013 m^3/ m^3 CH_4) [70].

Additionally, ammonium sulfate is stripped from the digestate (nutrient content according to [63]). Nitrogen stripping efficiency is 80% [71]. Afterwards the digestate is dewatered through centrifugation and subsequently dried to a DM content of 20%. The resulting thickened digestate still contains nutrients and can thus be used as a fertilizer. Thickening requires 0.69 kWh electricity/ t digestate treated in a decanter and 1.16 MJ heat/ kg of water that is evaporated in a two-step evaporation column [72].

The production of 2G ethanol from wheat straw as well as biogas provision from the remaining stillage presents a challenge that has not been realized at a fully competitive industrial scale yet. Therefore conversion efficiencies and process data considered here present an estimation of possible future lignocellulosic ethanol production according to the level of technology expected in 2020.

Similarly to 1G ethanol, ethanol is transported 150 km by truck from the production facility to the depot and another 150 km to the filling station [56].

Table 2 Inventory data for 2G ethanol production from wheat straw.

Concept **Fermentation** **Co-product**				**I** **C6** **feed**	**II** **C6** **biogas**	**III** **C5 & C6** **feed**
Input	Straw	kg		7.09	7.09	4.68
	Water	kg		8.07	13.90	5.93
	Enzymes	kg	[52,59]	0.05	0.05	0.03
	Corn steep liquor	kg	[60]	0.06	0.06	0.06
	DAP	kg	[60]	0.01	0.01	0.01
	Heat	MJ		31.27	25.13	20.84
	Pre-Treatment		*[73]*	*11.89*	*11.89*	*7.85*
	Distillation		*[73]*	*6.00*	*6.00*	*6.00*
	Molasses thickening		*[38]*	*13.38*		*6.99*
	Digestate thickening		*[38]*		*7.24*	
	Electricity	kWh		1.45	1.61	1.00
	Pre-Treatment		*[73]*	*0.35*	*0.35*	*0.23*
	Ethanol production		*[73]*	*0.98*	*0.98*	*0.65*
	Biogas production		*[74]*		*0.02*	
	Digestate thickening		*[72]*		*0.03*	
	Pressure swing adsorption		*[56]*		*0.10*	
	CO_2 capturing		*[55]*	*0.11*	*0.11*	*0.11*
	Electricity	MJ		0.60		0.21
Output	Ethanol	kg		1.00	1.00	1.00
	C5-Molasse, 60% DM	kg		2.89		1.01
	Stillage to biogas	kg			*14.57*	
	Lignin to energy generation	kg		*1.85*	*1.85*	*1.24*
	Biogas	MJ			9.78	
	Electricity	MJ			5.07	
	Digestate, 20% DM	kg			5.74	
	Ammonium sulfate	kg N			0.02	
	Wastewater	kg		9.94	6.32	5.50
	Direct emissions				*see Table 1*	
Parameter	Efficiency of energy generation			0.80	0.80	0.80

Thermal efficiency	0.71	0.56	0.70
Electric efficiency	0.10	0.24	0.10

4.2 Consequential system model

In the consequential approach, the effect of an introduction of 2G ethanol from wheat straw is assessed based on two scenarios:

1) the additional production of 2G ethanol from wheat straw; and
2) the shift from 1G ethanol to 2G ethanol.

In these cases, ethanol production takes place in Germany. Therefore, market data for the evaluation of occurring substitution effects refers to the respective markets in Germany. A basic assumption is that the German/European ethanol market is saturated. This assumption is justified by the existence of a blending rate that ties ethanol demand to fossil fuel consumption and by the fact that ethanol exports from the European Union increased slightly in recent years [75]. The quantity of ethanol to be blended with a fossil fuel depends on GHG savings according to the RED methodology of the respective provision concept and the envisaged reduction of GHG emissions of the fuel blend (section 3.1).

4.2.1 Business as usual scenario

The business as usual (BAU) scenario describes 1G ethanol production from wheat grains. (Figure 2). The process yields ethanol, DDGS, electricity and compressed CO_2. Ethanol is blended with gasoline according to the GHG savings achieved by the RED methodology in order to achieve a 6% reduction in GHG emissions from fuel provision and use.

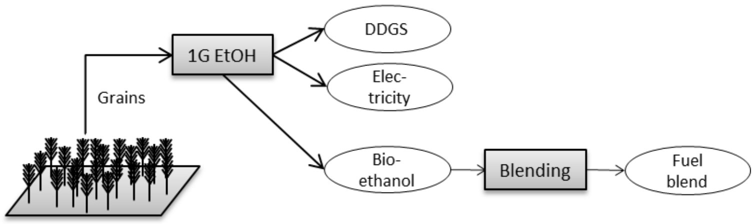

Figure 2 Business as usual (BAU) scenario. Captured CO_2 is not depicted. Abbr.: DDGS – dried distiller grains with solubles, EthOH – ethanol.

4.2.2 Scenario 1 "1G and 2G ethanol"

Scenario 1 describes the simultaneous production of 1G and 2G ethanol (Figure 3). The production of 1G ethanol takes place analogously to the BAU scenario. Additionally, straw is removed resulting in a change in SOC as well as a removal of nutrients. The latter are replaced by mineral fertilizer resulting in additional emissions. The methodological approach to assess the change in SOC and LUC is described in section 3.2.2. Product-specific substitution mechanisms as well as related emission estimations from LUC are described in Table 3 and Table 4. Alternative LUC scenarios are assessed in the sensitivity analysis.

The mixture of 1G and 2G ethanol results in higher GHG savings based on the RED methodology. Consequently, a lower quantity of fuel is blended to achieve the envisaged reduction in GHG emissions by 6%, as mandatory by 2020. The required quantity of ethanol to be blended is based on the average GHG saving of 1G ethanol and the respective 2G production concept. Surplus ethanol is assumed to be exported and to replace fossil fuel.

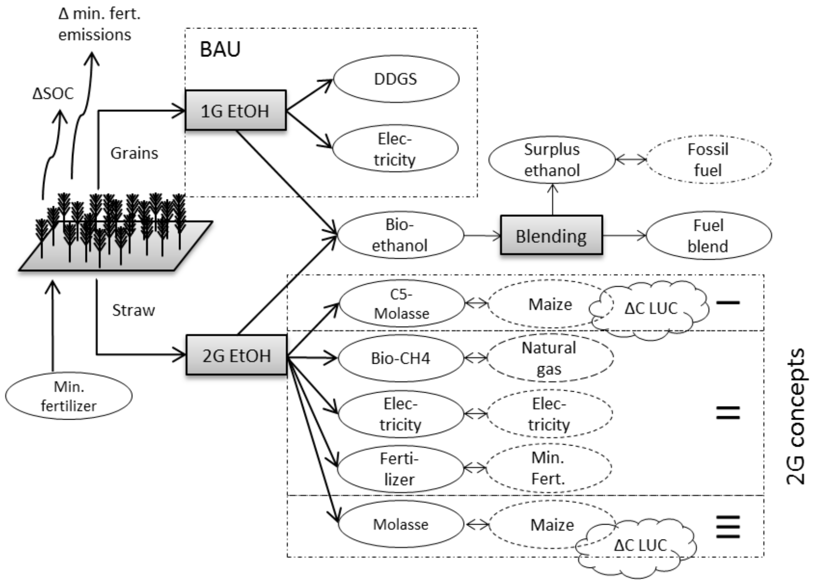

Figure 3 Scenario 1 "1G and 2G ethanol" (three concepts of 2G ethanol production are assessed (section 4.1.3); solid ellipses present products and dashed ellipses present substitutes of these products whose markets are affected (affected processes are not shown, Table 3); clouds indicate changes in land use that are considered (Table 4). Captured CO_2 and substitution mechanisms of the BAU scenario are not depicted. Abbr.: BAU – business as usual scenario, DDGS – dried distiller grains with solubles, EthOH – ethanol, LUC – land use change, min. fert. – mineral fertilizer, SOC – soil organic carbon.

4.2.3 Scenario 2 "Shift from 1G to 2G ethanol"

Scenario 2 describes a complete shift from 1G to 2G ethanol (Figure 4). As a consequence 1G ethanol is no longer produced and thus DDGS, compressed CO_2 and electricity from this process are no longer supplied to the market. Therefore, these missing products have to be provided by substitutes (Table 3). As in scenario 1, surplus bioethanol becomes available as a consequence of the shift from 1G to 2G ethanol due to the blending regulation based on GHG savings according to the RED. Two possibilities concerning how this surplus ethanol can be used are considered here: replacement of fossil fuels (scenario 2.1) and additional replacement of 1G ethanol (scenario 2.2). The choice of LUC scenarios and entailed emissions are explained in Table 4. Substitution quantities and LUC emissions are calculated based on section 3.2. Alternative LUC scenarios are assessed in the sensitivity analysis.

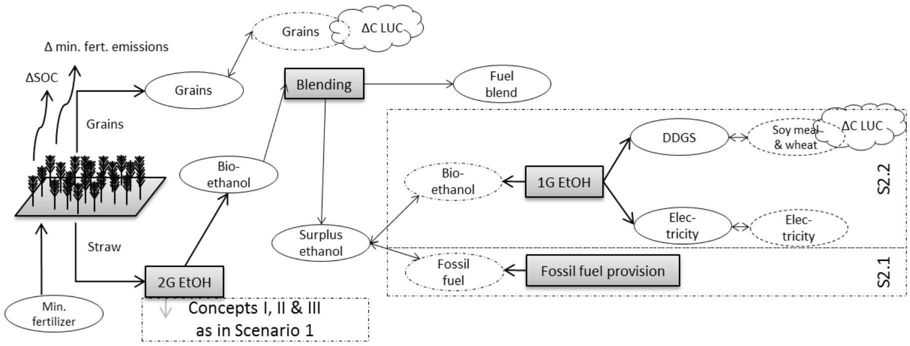

Figure 4 Scenario 2 "Shift from 1G to 2G ethanol" (as a consequence of the shift, 1G ethanol production is stopped; three concepts of 2G ethanol production are assessed (section 4.1.3). Solid ellipses present products and dashed ellipses present products whose markets are affected (affected processes are not shown, Table 3). Clouds indicate changes in land use that are considered (Table 4). Abbr.: EthOH – ethanol, LUC – land use change, min. fert. – mineral fertilizer, SOC – soil organic carbon.

Table 3 Substitution mechanisms.

Product (Scenario)	Substitution mechanism
Electricity (S1, S2)	In 2020, bituminous coal, will constitute a major part of the base and middle load supply in Germany [76]. 1G ethanol production and 2G concept II provide electricity. The lack of the former in scenario S2 and the existence of the latter in scenarios S1 and S2 result in a change in electricity supply. Due to the constant supply of electricity from ethanol facilities, electricity from bituminous coal is considered the marginal electricity.
DDGS (S2)	DDGS is substituted by a combination of protein feed and cereals. Vegetable oil completes the substitution mechanism (section 3.2.1). In Germany, 4 million t of rapeseed meal and 3.9 million t of soybean meal where fed to animals in 2015 [77]. The former showed an increase by 25% and the latter a decrease by 13% between 2011 and 2015 [77]. In the same period, imports of rapeseed meal to the EU and Germany increased by 39% and 98%, respectively, whereas soybean meal imports to the EU decreased by 16 % [78]. Rapeseed meal is a co-product of biodiesel production and its supply is predominantly controlled by biofuel production and not by feed demand. Consequently, it is assumed that DDGS is a substitute for soybean meal and vice versa. Additionally, wheat grains complement the nutrient and energy demand. In 2015, 55 % of soy meal in Germany was imported from Brazil, followed by the Netherlands (21%) and Argentina (19 %) [79]. In 2015, soy meal imported to the Netherlands predominantly originated from Brazil (57%), Argentina (45%) [77]. Thus, around 68 % of soybean meal used in Germany in 2015 originates from Brazil. In case of soybeans, 45 % came from the US and 39 % from Brazil. Between 2000 and 2014, developments in yields and planted areas indicate a stable development in the US, while yields and planted area of soybean increased considerably in Brazil (Figure S.3). It is therefore assumed that Brazil is the marginal supplier of soy. The majority of Brazilian soybean (meal) is exported from Paranaguá (36%), Santos (25%), Rio Grande (1%) and Vitória (8%) [80]. The averaged shipping distance from these ports to Hamburg, Germany, is 10,723 km. Palm oil presents the most used vegetable oil world-wide and the price of palm oil has been lower than that of rapeseed and soybean oil in the past 5 years [78,81,82]. Therefore it is assumed that palm oil is the oil that complements the feed substitution mechanism. The major exporters of palm oil are Indonesia and Malaysia, providing 49 % and 40 % of global palm oil exports in 2014/15, respectively [78]. Consequently, Indonesia and Malaysia supply 55% and 45% of palm oil to the European market (adjusted shares), respectively. In Indonesia, 96% of palm oil is produced in Sumatra (75%) and Kalimantan (21%) [83]. It is assumed that palm oil is shipped from Port Klang, Jakarta and Pontianak in case of production in Malaysia, Sumatra and Kalimantan, respectively. The averaged shipping distance to Hamburg, Germany, is 13,958 km. Subsequently road transport via trucks for another 300 km is assumed for soybean meal and palm oil.
Molasses (S1, S2)	Molasses, a co-product from 2G concepts I and III, is assumed to substitute maize based on the metabolizable energy. Maize is assumed to be cultivated in Germany as 85 % of domestic maize consumption is provided by domestic production [84]. Maize is assumed to be transported 300 km by truck.
Biomethane (S1, S2)	Biomethane, a product of 2G concept II, replaces the provision and combustion of the equivalent amount of natural gas.
Fertilizer (S1, S2)	Thickened digestate and ammonium sulfate, co-products of biogas production of 2G concept II, replace mineral fertilizer according to their nutrient content. A transport distance of 300 km is assumed.
Wheat grains (S2)	In scenario S2, wheat grains become available due a shift from 1G to 2G ethanol and needs to be supplied due to missing DDGS as part of the DDGS replacement scheme (section 3.2.1). Wheat is assumed to be transported 300 km by truck.
Ethanol (S2)	Surplus ethanol as a consequence of blending regulation is either exported whereby it replaces fossil gasoline provision and use (S1, S2.1), or substitutes 1G ethanol in Germany (S2.2). The fuel efficiency of (low) fuel blends, as currently common in the EU, is considered equal to that of pure gasoline [85].
CO_2 (S1, S2)	Captured CO_2 is assumed to replace fossil derived CO_2.

Table 4 Land use change mechanisms and related carbon stock changes over 20 years.

Mechanism (Location)	**Description and parameters (Eq. 10)**
Straw removal (Germany)	The sustainable straw potential is 44.7% of the overall available straw. Straw is harvested and processed according to section 2.2 of the supplementary material. The assumed soil is a Luvisol / Avisol ($\boldsymbol{SOC_{REF} = 95\ t/ha}$) [41]. The cultivation system is a long-term cultivation in moist temperate climate with full tillage ($\boldsymbol{F_{LU}}$ = 0.69, $\boldsymbol{F_{MG}}$= 1, $\boldsymbol{C_{veg_{0-T}} = C_{veg_0} = 0\ t/ha}$). All of organic input is converted to carbon if straw is not removed ($\boldsymbol{F_I}$ = 1); if straw is removed, 92% are converted ($\boldsymbol{F_I}$ = 0.92). Straw removal results in a C loss of 0.26 t C/ (ha a).
Conversion from / to cropland (Germany)	In scenario 2, wheat grains become available and reduce domestic wheat production. Additional wheat is required to substitute missing DDGS. The corresponding LUC is a conversion from or to fallow land ($\boldsymbol{F_{LU}}$ = 0.82, $\boldsymbol{F_{MG}}$= 1.1, $\boldsymbol{F_I}$= 0.95, $\boldsymbol{C_{veg_0} = 6.8\ t/ha^a}$) [41]. An alternative LUC mechanism is assessed in the sensitivity analysis.
Soybean cultivation (Brazil)	In 2013/14, 52% of Brazilian soy was cultivated in the Central West and 27% in the South [86]. Between 2001 and 2005, the expansion of land used for soy cultivation took place on rainforest land (26%) and on scrubland (74%) [87]. In the subsequent four years, the conversion occurred mainly on scrubland (91 %). Only 22% of increasing demand was fulfilled by intensification, whereas the rest was provided by extensification [87,88]. Thus, it is assumed that this trend continues and that, consequently, land conversion for soy cultivation occurs on scrubland/ grassland; this also reflects the current Brazilian policy, e.g. Plano de Ação para Prevenção e Controle do Desmatamento na Amazônia Legal (PPCDAm). It is assumed that soy cultivation takes place in Central-West Brazil on low activity clay soils ($\boldsymbol{SOC_{REF} = 47\ t/ha}$) [41,80,89]. Soy is cultivated in a full-tillage system with medium inputs ($\boldsymbol{F_{LU}}$ = 0.48, $\boldsymbol{F_{MG}}$ = $\boldsymbol{F_I}$ = 1, $\boldsymbol{C_{veg_0} = 0\ t/ha}$) [41,89]. It is assumed that an averagely degraded savanna is converted ($\boldsymbol{F_{MG}}$ = 0.97, $\boldsymbol{F_{LU}}$ = $\boldsymbol{F_I}$ = 1, $\boldsymbol{C_{veg_{0-T}} = 53\ t/ha}$). The conversion results in C loss of 3.8 t C/ (ha a). Other LUC mechanisms and cultivation practices are assessed in the sensitivity analysis.
Oil Palm cultivation (Indonesia)	In Indonesia, forest cover decreased from 130 million ha in 1975 to 91 million ha in 2005. About half of this decrease can be attributed to palm oil plantations [90]. In Sumatra and Kalimantan, where 95% of total land used for palm oil cultivation in Indonesia is located and 96% of Indonesian palm oil is produced. In these areas annual forest cover loss is 2.5%; this is significantly higher than the overall level in Indonesia (1.9%) [83,90]. Forest land presents the land use category with the largest decreases, while others, e.g. permanent pastures, decreased to a much lower extent in absolute terms. It is therefore assumed that insular native forest is converted ($\boldsymbol{F_{LU} = 1}$, $\boldsymbol{C_{veg_{0-T}} = 230\ t/ha}$) to palm oil plantations ($\boldsymbol{F_{LU}}$ = $\boldsymbol{F_{MG}}$ = $\boldsymbol{F_I}$ = 1, $\boldsymbol{C_{veg_0} = 60\ t/ha}$) [41]. A low activity clay soil is assumed ($\boldsymbol{SOC_{REF} = 60\ t/ha}$). The conversion results in C loss of 8.5 t C/ (ha a). Note: In 2016, a five-year moratorium on new palm plantations was issued. It prohibits the establishment of new plantations on forest land. A conversion of permanent cropland to oil palm plantations and the establishment of a plantation on peatland in Indonesia is assessed in the sensitivity analysis.
(Malaysia)	Historical data from 1989 to 2013 shows that deforestation and oil palm expansion show similar growth patterns [91]. Oil palm cultivation showed an expansion from 0.1 to 5.5 million ha between 1975 and 2005. During the same period, forest land and other permanent crops showed a large decrease by 4.6 and 1.4 million ha, presenting a decrease by 20 and 45 %, respectively [90]. It is therefore assumed that 76.7 % of land conversion to palm oil plantations ($\boldsymbol{F_{LU}}$ = $\boldsymbol{F_{MG}}$ = $\boldsymbol{F_I}$ = 1, $\boldsymbol{C_{veg_{0-T}} = 60\ t/ha}$) takes place on continental forest land ($\boldsymbol{F_{LU} = 1}$, $\boldsymbol{C_{veg_{0-T}} = 185\ t/ha}$) while the remaining 23.3% takes place on permanent crop land ($\boldsymbol{F_{LU}}$ = $\boldsymbol{F_{MG}}$ = $\boldsymbol{F_I}$ = 1, $\boldsymbol{C_{veg_{0-T}} = 34.3\ t/ha}$) [41,90]. A low activity clay soil is assumed ($\boldsymbol{SOC_{REF} = 60\ t/ha}$). This results in C loss of 4.5 t C/ (ha a). In the sensitivity analysis, a complete conversion of permanent crops, e.g. rubber, to palm oil plantations as well as the establishment of plantations on peatland is assessed.
	[a] The C content of grassland is taken to estimate the C content in set-aside land.

5. Results and discussion

First, GHG savings[2], determined by the RED methodology are presented. These values serve as an input to consequential assessment: GHG savings calculated with the RED methodology determine the quantity of biofuel to be blended with a fossil fuel. In the year of reference, 2020, the fuel mixture needs to reduce GHGs by 6 % compared to the baseline of 94.1 g CO_{2eq}/MJ [33]. GHG intensities of processes and substitutes as well as emissions from LUC can be found in Table S.3 and Table S.4. A brief summary of the sensitivity analysis is presented in the following chapters. The detailed sensitivity analysis is presented in section 3.3 of the supplementary material. All presented results rely on the assumptions previously presented.

5.1 GHG savings according to the RED methodology

Results and discussion. All assessed 1G and 2G concepts reach the required GHG savings of at least 50% (Figure 5): 1G and 2G ethanol production with the production concepts I, II and III result in GHG emission savings of 57, 103, 105 and 103%, respectively.

In the case of 1G ethanol production, the largest contributor to the GHG emissions are wheat cultivation and transport with about 34 g CO_2-eq./MJ ethanol[3]. Ethanol production and co-product processing, i.e. stillage drying, results in 21 g CO_2-eq. /MJ ethanol. Thereof, 95 % originate from energy provision by natural gas. The remaining GHG emissions stem from the provision of auxiliary materials. CO_2 capture and surplus electricity result in a credit of 20 g CO_2-eq. /MJ ethanol, whereof electricity accounts for 2.3%.

In case of 2G ethanol, concept III results in highest savings. This is due to the co-fermentation C5- and C6-sugars and thus lower energy and feedstock requirements per fuel output. Straw is considered a residue and thus its cultivation is not considered by the RED methodology, except for its handling and transport. GHG emissions from straw handling and transport activities range from 2 to 3 g CO_2-eq./ MJ ethanol. In case of lignin-fired energy generation, non-CO_2 emissions, e.g. N_2O, play the most important role.

Sensitivity analysis. The sensitivity analysis reveals that the magnitude of change in GHG savings is lower than the magnitude of a change in energy (heat) demand of 1G and 2G ethanol production (Fig S.4). A change in conversion efficiency has an even smaller effect on GHG savings according to RED methodology (Fig S.5).

[2] The terminology „*GHG savings*“, here and hereafter, refers to the value calculated by RED methodology (Eq. 1) and does not reflect occurring reductions in GHG emissions due to the introduction and use of biofuels (see section 3.1).
[3] All reported values present results after allocation based on the LHV, if not stated otherwise.

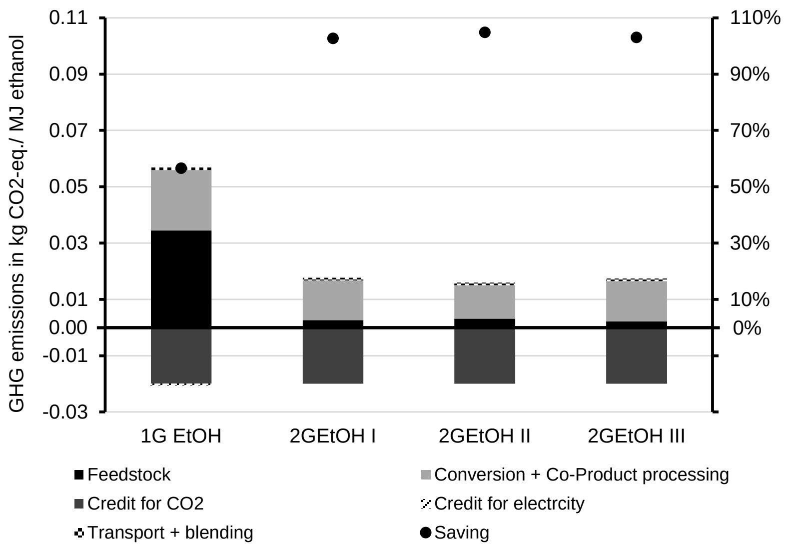

Figure 5 GHG emissions (left axis) and GHG emission savings (right axis) according to RED methodology (EtOH – ethanol).

5.2 The consequential approach: From 1G to 2G ethanol

Results and discussion. Based on GHG savings according to RED methodology, 98, 61, 63 and 62 MJ of ethanol needs to be blended with gasoline per GJ of fuel blend in case of 1G, 2G concepts I, II and III, respectively, in order to achieve the envisaged GHG reduction of 6%. Accordingly, 32660 GJ of fuel energy each containing 98 MJ ethanol, can be supplied by the 1G ethanol facility with an annual capacity of 150,000 m³ (BAU scenario). The absolute quantity of fuel blend to be sold on the market is not affected by the shift from 1G ethanol to 2G ethanol, whereas the quantity of ethanol required to be blended with fossil fuel changes according to GHG savings according to RED methodology and the envisaged reduction in GHG emissions by 6%. All surplus ethanol that is not required to supply these 32660 GJ is either exported where it replaces fossil fuel energy (scenarios 1 and 2.1) or it substitutes domestic production of 1G ethanol (scenario 2.2). Results indicate that the introduction of 2G ethanol leads to a decrease in GHG emissions if 2G ethanol is additionally produced to 1G ethanol (scenario 1, Figure 6). The decrease ranges from 9.0 to 12.1 kg CO_2-eq./ GJ fuel blend. 2G ethanol production combined with biogas production (2G concept II) results in highest decreases due to credits for the substitution of natural gas provision and combustion by biomethane as well as due to surplus electricity generation substituting electricity in the market (Table 3). Molasses, a co-product of the other two concepts, results in a small decrease in GHG emissions due to the replacement of maize. The largest contributions to emission savings, in total around 13 kg CO_2-eq. /GJ fuel blend, stem from the replacement of fossil fuels due to the saturated market conditions, the doubling of production capacities in scenario 1 and the assumption of a substitution of fossil fuels by surplus ethanol. Thus, results of scenario 1 rely on the assumption that surplus ethanol fully substitutes fossil fuels. Additionally, the quantity of captured CO_2 doubles. Moreover, the likewise amount of fossil derived compressed CO_2 is replaced.

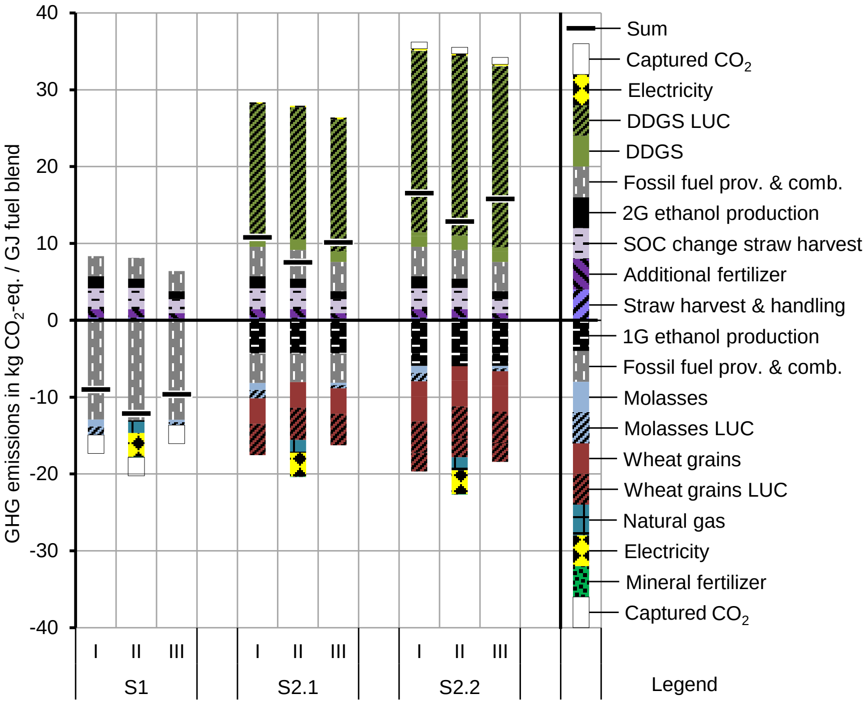

Figure 6 Changes in GHG emission due to the introduction of 2G ethanol per GJ fuel blend (a total of 30644 GJ fuel blend is supplied to the market based on the BAU scenario. Roman numbers denote 2G concepts according to section 4.1.3. Abbr.: DDGS – dried distiller's grains with solubles, LUC – land use change, SOC – soil organic carbon.

The shift from 1G to 2G ethanol (scenario 2) results in an increase in GHG emissions. This increase ranges from 7.5 to 10.8 and from 12.9 to 16.5 kg CO_2-eq./ GJ ethanol in case of a replacement of fossil fuel (scenario 2.1) and in case of a replacement of 1G ethanol (scenario 2.2) by surplus ethanol, respectively. The surplus in scenario 2 originates from lower blending requirements as a consequence of higher GHG savings according to the RED requirements. In case surplus ethanol replaces 1G ethanol, the respective co-products from 1G ethanol need to be provided by other substitutes (i.e. feed, CO_2 and electricity, Table 3).

As an additional consequence of shifting production from 1G to 2G ethanol is that DDGS and electricity are no longer supplied through this process. The provision of feed replacing DDGS results in emissions of around 25 kg CO_2-eq./ GJ ethanol, of which 93% stem from LUC (Figure 7). The largest contributors are soy cultivation and related LUC. This is due to relatively low yields and high carbon stock changes. The sum of emissions related to the substitution of feed products is around 14 kg CO_2-eq./ GJ ethanol. The provision of feed is a major reason for an increase in emissions if 1G being replaced by 2G ethanol. Consequently, the provision of feed entailing lower emissions presents a major lever to reduce negative effects if political targets are put into practice.

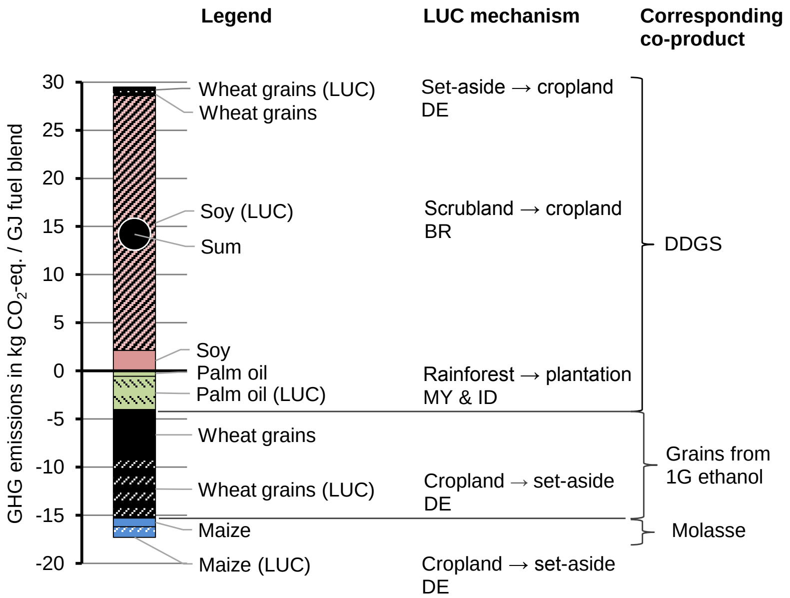

Figure 7 GHG emissions from agricultural production and LUC of substitutes of 2G ethanol production concept I (scenario 2.2). Abbr.: DDGS – dried distiller's grains with solubles, DE – Germany, ID – Indonesia, LUC – land use change, MY – Malaysia.

These outcomes are highly relevant in the context of the current ongoing revision of the RED: the proposed reduction of the share of 1G biofuels and increase of the share of 2G biofuels will eventually trigger the replacement of the former by the latter (if the absolute energy demand in the transportation sector decreases as predicted) [6]. Thus, proposed legislation might trigger an increase in emissions. The magnitude of the increase in emissions is emphasized by the fact that certain 2G biofuels are at an advantage in the revised RED by considering their provision carbon-neutral up to the point of their collection, thereby resulting in higher GHG savings. Past works confirmed that this is not justifiable from a scientific point of view, cf. [23,24]. As a consequence of an additional lowering of GHG savings, higher quantities of 1G fuel will be displaced by lower quantities of 2G biofuel resulting in higher shares of fossil fuels contained in the fuel blend.

Based on these findings, two options are given to prevent or lower an increase in emissions due to the introduction of 2G fuels. Firstly, legislation should promote the production of 1G and 2G ethanol and ensure the displacement of fossil fuel (scenario 1). It should be noted that this does not imply an increase in production of 1G ethanol. Secondly, if the replacement of 1G by 2G ethanol is turned into practice as proposed, protein feed entailing low GHG emissions should be supplied from land that becomes available to prevent iLUC.

Sensitivity analysis. The sensitivity analysis shows that a change in heat demand or a change in conversion efficiency only slightly affects changes in emissions due to the simultaneous production of 1G and 2G ethanol or due to the shift from 1G to 2G ethanol (Figures S.4 and S.5). Apart from a change in GHG savings as a key input parameter of the consequential approach, a change in heat demand and conversion efficiency affect the quantity of co-products that are provided, i.e. electricity and molasses. In certain cases, an increase in energy demand or a decrease in conversion efficiency will even lead to a (minor) decrease in emissions compared to the reference case. A change in GHG savings ranging from -15 to + 15% without a change in the quantity of co-products, e.g. due to a change in emissions from feedstock provision, results in a maximum relative change in results by 40% and a maximum absolute change in results by 2.8 kg CO_2-eq./GJ fuel blend (Figure S.6). Within the assessed range of changes in parameters, emission decreases (scenario 1) and emission increases (scenario 2) remained a decrease and an increase in emissions, respectively.

Emissions from LUC contribute a large extent to emissions (Figure 6 and Figure 7). The assessment of alternative LUC variants shows that:

- The increase in GHG emissions due to a shift from 1G to 2G ethanol will be lower, if land that becomes available due to the availability of wheat grains in scenario 2 turns into forest and settlement area. Such a land-use change was observed in Germany between 2004 and 2014. The change in emissions ranges from 2 to 23% (Figure S.7).
- A change in cultivation practice of soybean (reduced or no-tillage) has only a minor effect on results (Figure S.8).
- A change in cultivation location and biome where LUC of soybean cultivation occurs can result in lower emissions than in the reference case. If moderately or severely degraded savanna is converted to soybean plantations in Southern Brazil, scenarios 2.1 and 2.2 will result in a (slight) decrease in overall emissions. In recent years, extensification of agricultural land has slowed in Brazil. However, in the Central West, where most of Brazilian soy is cultivated, extensification and intensification took place in parallel [88,92]. Assuming that no LUC occurs, emissions will be reduced by a larger extent (Figure S.8).
- The conversion of peat land or native forest to oil palm plantations results in high LUC emissions. However, recent trends observed in Malaysia, as well as the moratorium on new oil palm plantations that was passed in Indonesia, indicate that LUC mechanisms might change. A change in LUC mechanisms of oil palm cultivation results in an increase in overall emissions if less CO_2 is emitted by the land conversion (Figure S.9). This is due to the fact that soy bean feed, that needs to be supplied as a consequence of a shift from 1G to 2G ethanol production, supplied oil to the market. This oil is assumed to reduce the demand for palm oil. Thus, the decrease in emissions attributed to the system are lowed, if emissions entailed to the provision of palm oil are lower than assumed in the reference case.

Caveat: in case the substitution effects are too small to trigger changes in palm oil demand (due to low oil quantities of soy beans and low shares of DDGS in the overall feed market), the increase in emissions due to shift from 1G to 2G ethanol ranges from 20 to 28% among all concepts and scenarios.

Limitations. The assessment of consequences as a result of changes in production patterns requires the consideration of substitution mechanisms and changes in market behavior. Several aspects are not or only partially covered in this study, e.g.:

- The production of 2G ethanol from wheat straw as well as biogas from remaining stillage presents a challenge and has not been realized at a competitive scale yet.
- No decrease in grain yield due to straw harvest was assumed.
- No rebound effect of fossil fuel prices and resulting change in demand is considered. Other studies indicate a substantial rebound effect, cf. [93].
- The change prices of commodities will affect supply and demand of products and co-products.
- In certain cases average production data (e.g. yield) is used. The marginal change in production might result in different conditions.

- A simplified model is applied to account for LUC and related emissions, which are part of a complex global agricultural commodity system: where and to what extent LUC, extensification and intensification occurs is estimated by a deterministic model.

The assessed scenarios could therefore be considered to present two extremes: In scenario 1, it is assumed that surplus ethanol fully replaces fossil fuel and in scenario 2, it is assumed that the demand for protein feed will be fully met by soybean meal and wheat grains stimulating agricultural expansion.

6. Conclusion

The current paper demonstrates how the introduction of novel liquid biofuels can be assessed in the context of the European legislation to support robust decision-making. Future studies can built thereupon and expand the analysis by including other fuels and extend the understanding of potential market mechanisms. A generalized framework that is valid in the context of the European legislation and markets and that can be applied to all fuel and mobility concepts, e.g. for biofuels and e-mobility alike, should be developed.

Under the given assumptions, the simultaneous production of 1G and 2G ethanol results in a decrease in emissions if surplus ethanol (from a doubling of production capacities plus minor surplus quantities due to blending regulations) replaces fossil fuels elsewhere. In contrast, the shift from 1G to 2G ethanol might increase GHG emissions:

- Emissions increase regardless of the 2G concept. The choice of the production concept of 2G ethanol is not of high importance regarding total changes in emissions that are triggered. Even higher conversion efficiencies or lower energy requirements do not change these findings.
- Direct emissions from 2G ethanol production play a minor role in comparison to changes in GHG emissions due to occurring substitution mechanisms. This is the case, if 1G ethanol is replaced by 2G ethanol under given assumptions: the provision of protein feed that is required to supply the market demand for feed might increase emissions. The largest source of emissions is LUC. The negative LUC emissions resulting from the occurring availability of wheat grains are, by far, outweighed by LUC emissions entailed to the supply of protein feed.
- A shift from a fuel with relatively low GHG savings (here: 1G ethanol) to a fuel with higher savings (here: 2G ethanol concepts) results in lower quantities of biofuel to be blended with fossil fuel and thus, higher quantities of fossil fuel contained in the blend.

It can be concluded, that the existing terminology “GHG savings”, as defined by the RED, is misleading: according to the RED’s terminology, 2G ethanol results in a decrease in GHG emissions, but the analysis of consequences of an introduction of 2G ethanol shows the opposite. The application of the RED methodology can serve the purpose of certification as it might give an indication of concepts emitting low emissions in the production phase but the methodology does not reflect occurring changes in emissions triggered by substitution mechanisms as a consequence of the introduction of a novel fuel. The analysis of these effects reveals that an increase in emissions might be triggered. The revised RED will eventually shape the European (and global) biofuel industry for the upcoming decades. The current draft of the RED indicates that mechanisms similar to those assessed in the current work will be promoted if total energy demand in the transport sector decreases. It can be concluded, that the new RED, if turned into practice as proposed, might not facilitate a reduction in GHG emissions while falsely claiming to do so.

A change in the demand for biofuels affects global food and feed markets and legislation should therefore target emissions (and other effects) of agricultural commodities in general, independently from their use as food, feed, fiber or fuel in order to avoid a shift of emissions from one market (e.g. biofuels) to another (e.g. feed). Likewise, a reduction in absolute GHG emissions can only be achieved by the coordination of concepts serving the needs for food, feed, fiber and fuel. It is therefore suggested to develop legislation that comprehensively addresses these demands and promotes those production concepts that entail lowest emissions while contributing to the fulfillment of the demands.

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Supplementary material

Changes in greenhouse gas emissions due to the introduction of wheat straw ethanol in the context of European legislation: A consequential GHG assessment

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Table of Contents

1 Methodology

1.1 Global warming potentials

Table S.1 Global warming potentials according to the RED [1] and IPCC [2].

Substance	RED	IPCC 2013
Carbon dioxide, fossil	1.0	1.0
Carbon dioxide, from soil or biomass stock	1.0	1.0
Carbon monoxide, biogenic		2.5
Carbon monoxide, fossil		4.1
Carbon monoxide, from soil or biomass stock		4.1
Chloroform		16.4
Dinitrogen monoxide	296.0	264.8
Ethane, 1,1,1,2-tetrafluoro-, HFC-134a		1301.3
Ethane, 1,1,1-trichloro-, HCFC-140		160.1
Ethane, 1,1,1-trifluoro-, HFC-143a		4804.4
Ethane, 1,1,2-trichloro-1,2,2-trifluoro-, CFC-113		5823.7
Ethane, 1,1-dichloro-1-fluoro-, HCFC-141b		782.0
Ethane, 1,1-difluoro-, HFC-152a		137.6
Ethane, 1,1-difluoro-, HFC-152a		137.6
Ethane, 1,2-dichloro-		0.9
Ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-, CFC-114		8592.2
Ethane, 1-chloro-1,1-difluoro-, HCFC-142b		1982.0
Ethane, 2,2-dichloro-1,1,1-trifluoro-, HCFC-123		79.4
Ethane, 2-chloro-1,1,1,2-tetrafluoro-, HCFC-124		526.5
Ethane, chloropentafluoro-, CFC-115		7665.4
Ethane, hexafluoro-, HFC-116		11123.5
Ethane, pentafluoro-, HFC-125		3169.3
Methane, biogenic	23.0	28.5
Methane, bromo-, Halon 1001		2.4
Methane, bromochlorodifluoro-, Halon 1211		1746.5
Methane, bromotrifluoro-, Halon 1301		6291.6
Methane, chlorodifluoro-, HCFC-22		1764.6
Methane, chlorotrifluoro-, CFC-13		13893.4
Methane, dichloro-, HCC-30		8.9
Methane, dichlorodifluoro-, CFC-12		10239.2
Methane, dichlorofluoro-, HCFC-21		147.7
Methane, difluoro-, HFC-32		676.8
Methane, fossil	23.0	29.7
Methane, from soil or biomass stock	23.0	29.7
Methane, monochloro-, R-40		12.2
Methane, tetrachloro-, R-10		1728.5
Methane, tetrafluoro-, R-14		6625.8
Methane, trichlorofluoro-, CFC-11		4662.9
Methane, trifluoro-, HFC-23		12397.6
Nitrogen fluoride		16070.0
Pentane, perfluoro-		8546.7
Sulfur hexafluoride		23506.8

1.2 Feed as a co-product: feed and oil substitution

Dried distiller's grains with solubles (DDGS) substitutes protein feed and cereals (equations (7) and (8)). The provision of such a protein feed meal is coupled to vegetable oil production. When meal is substituted, oil production is reduced and needs to be supplied from other suppliers. This can be expressed by a converging series (Eq. (S.1 and S.2) and Figure S.1)

$$P_{meal} = \sum_{i=0}^{n} a(\frac{m}{o})^n \Rightarrow P_{meal} = \lim_{n\to\infty} \sum_{i=0}^{n} a(\frac{m}{o})^n \Rightarrow P_{meal} = \frac{a}{1-{m}/{o}} \text{ for } {m}/{o} < 1 \quad \text{(S.1)}$$

$$P_{oil} = \sum_{i=1}^{n} a(\frac{m}{o})^n \Rightarrow P_{oil} = \lim_{n\to\infty} \sum_{i=1}^{n} a(\frac{m}{o})^n \Rightarrow P_{oil} = \frac{a\ {m}/{o}}{1-{m}/{o}} \text{ for } {m}/{o} < 1 \quad \text{(S.2)}$$

Where P denotes protein production substituted by the feed co-product (P_{meal}) and the production of protein that is coupled to oil production (P_{oil}). m and o denote the oil content per protein and a denotes the starting quantity of protein that is substituted.

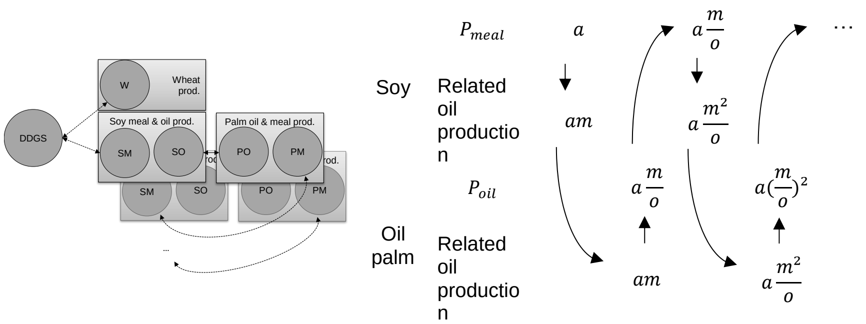


Figure S.1 Depiction of substitution mechanisms (left) and its mathematical representation (right). Abbr.: DDGS – dried distiller's grains with solubles, PM – Palm kernel meal, PO – palm oil, SM – Soy meal, SO – Soy oil, W - Wheat. Adapted from [3].

Integrating equations (S.1) and (S.2) into the linear system of equations (7) and (8) allows the calculation of the appropriate amount of feed that is substituted while accounting for the metabolizable energy, digestible protein, as well as occurring feedback loops.

2 System description

2.1 Sustainable straw potential

According to Weiser et al. [4], the quantity of straw that can be sustainably extracted from an agronomic system is mainly dependent on the consequences on soil humus. Soil humus provides nutrients, stores water, filters drainage water and shows a high biological activity [5,6]. All these factors are of crucial importance for healthy ecosystems and therefore for agricultural production as well. As straw removal affects the soil humus reproduction, the quantity of straw that can be sustainably removed restricts the technical straw potential [4]. Thus, the sustainable amount of straw that can be harvested can be determined by the standard humus balance method developed for Germany by the Associations of German Agricultural Analytic and Research Institutes (equation (S.3)) [5].

$$Soil\ humus = Input\ of\ humus - humus\ demand \quad \text{(S.3)}$$

In order to avoid humus loss, the soil humus balance should equal zero [4]. The input of humus and the humus demand depend on endapho-climatic conditions. The factors to be applied in the standard method are based on decades of measurements in Germany (6 sites), Sweden (2), Czech Republic (1), Denmark (1), Poland (1) the UK (1) [7]. At these sites, sand, loamy sand, sandy loam, loam/clay and chernozem soils can be found. The mean temperature at these sites ranges from 5.5 (Sweden) to 10°C (Germany). The average annual precipitation ranges from 484 (Germany) to 790 (Denmark). The humus demand of cereal cultivation ranges from 280 to 400 kg C/(ha a) [5,7]. The lower value is chosen, as it represents soils with adequate supply of nutrients and soil in good conditions [5]. The reproduction of soil humus from wheat straw is 80 to 100 kg C/(t substrate) [5]. In case of intensive agriculture, the reproduction is 80 kg C/(t substrate) [2]. The assumed grain yield is 7.9 t/(ha a) and the grain to straw ratio is 0.8 [8].

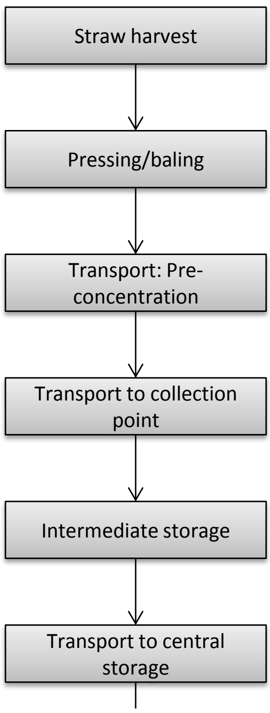
The soil humus balance without straw removal can be calculated based on equation (S.3) according to equation (S.4).

$$Soil\ humus_{no\ straw\ removal} = 80\ \frac{kg\ C}{t_{straw}} * 6.32\ \frac{t_{straw}}{ha\ a} - 280\ \frac{kg\ C}{ha\ a} = +225.6\ \frac{kg\ C}{ha\ a} \qquad (S.4)$$

The share of straw that can be removed can thus be calculated at 44.7 %. This calculation is comparable to other studies (e.g. [4]).

2.2 Straw handling

The handling and transportation of straw after harvest is modelled as follows.



Straw is harvested with a combine harvester. Life cycle inventory (LCI) data of straw harvest are based on Ecoinvent v3.2 process ‘combine harvesting’ [9,10].

Bale pressing is accomplished with a round baler. LCI of baling is based on Ecoinvent v3.2 process ‘baling, GLO’ [9,10].

Bales are collected for further transport. LCI of bale concentration is based on Ecoinvent v3.2 process ‘bale loading, GLO’[5, 6]. Assumed loss is 1 % [7].

Straw bales are transported to intermediate storages by tractors. LCI of transport is based on Ecoinvent v3.2 process ‘market for transport, tractor and trailer, agricultural, GLO’ [5, 6].

Bales are assumed to be stored covered with foil (60 %) or in a light structure storage building (40 %). The loss of material is 8 % in the former and 2 % in the latter [11].

Transport to the central storage facility is realized by heavy duty vehicles. LCI of transport is based on Ecoinvent v3.2 process ‘transport, freight, lorry >32 metric ton, EURO5, RER’[6]. Assumed loss is 1 % for transport as well as for handling [11].

The central storage facility is a storage hall in close proximity to the ethanol facility.

Transport of straw is modelled, assuming a rectangular quadratic area from where feedstock is sourced (Figure S.2). The total area, A_{total}, from which straw is collected, is calculated with equation (S.5).

$$A_{total} = \frac{\frac{S_d}{\prod(1-l_i)}}{S_a} \quad \text{(S.5)}$$

Where S_d describes the straw demand of the ethanol facility, l_i the losses at each processing step , and S_a the straw availability (adapted from [8]). Each intermediate storage facility is used to store straw from 9 parcels, measuring 20 ha each. The average availability of straw, S_a, is 0.27 t_{DM}/ha [7]. This value presents an estimation of the straw availability in Germany, based on the sustainable straw potential of 44 % and the total surface area.

The area of each intermediate storage, A_{is}, can be calculated based on equation (S.6).

$$A_{is} = \frac{A_{total}\, 180ha\, s_p}{\frac{S_d}{\prod(1-l_i)}} \quad \text{(S.6)}$$

Where s_p is the technical straw potential. The average distance from each parcel to the intermediate storage, realized by tractors, is calculated by the square root of A_{is}. The average distance from all intermediate storages to the central storage/ the ethanol facility, accomplished by heavy duty vehicles, is calculated by the square root of A_{total}.

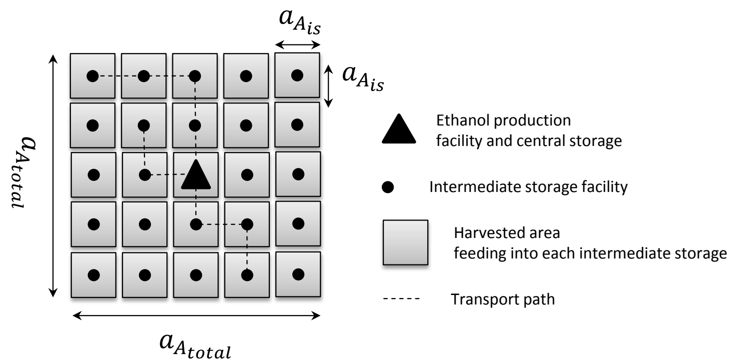


Figure S.2 Schematic depiction of modelled straw transport (adapted from [12])

2.3 Ethanol from wheat straw

Table S.2 Composition of solid and liquid phase and recovery rates of steam explosion of wheat straw at 190°C for 10 minutes [13].

Liquid Fraction	**g/100g raw material**	**Solid fraction**	**% of DM**
Glucose	3.1	Glucan	62.80%
Xylose	14	Xylan	13.10%
Galactose	1.4	Galactan	0.20%
Arabinose	2.2	Arabinan+ Mannan	0.80%
Mannose	0.2	Acid insoluble lignin	24.30%
		Ashes	2.80%
Inhibitors			
Furfural	0.09		
5-HMF	0.02		
Acetic acid	0.58		
Formic acid	0.34		
Vanillin	0.02		
Coumaric acid	0.02		
Ferulic acid	0.00		
Recovery rates			
Glucan recovery	97.95%		
Xylan recovery	91.10%		
Solid recovery	50.09%		

2.4 Substitution mechanisms

Yields and planted area of soy production have been stable in the US in recent years, while yields and planted area showed an increase in Brazil (Figure S.3). Therefore, Brazil is considered the marginal supplier of soybean (meal).

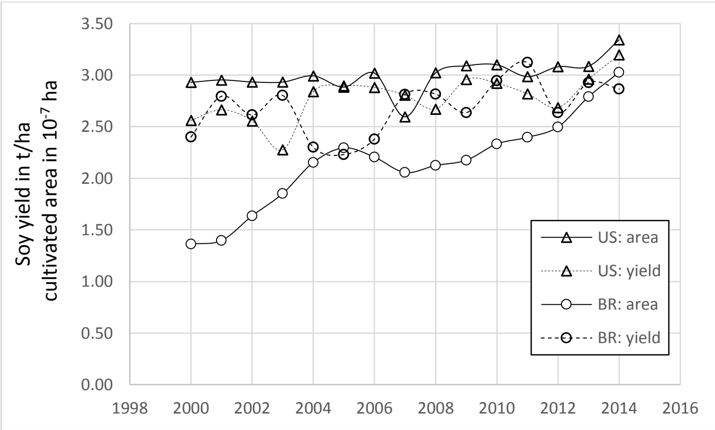


Figure S.3 Planted area and yield of soy production in Brazil (BR) and the United States (US) [14].

3 Results

3.1 GHG intensities

Table S.3 GHG intensities

	kg CO_2-eq./		
Petrol	kg	1.25	[10]
Petrol combustion	MJ	0.08	[15]
Rape meal	kg	0.91	[16]
Maize	kg	0.37	[16]
Palm fruits	kg	0.16	[16]
Electricity from coal	MJ	0.29	[10]
Natural gas provision	m3	0.41	[10]
Natural gas combustion	MJ	0.06	Own calculation
Additional fertilizer	kg straw removed	0.06	[10]
Soybean meal	kg	0.51	[16]
Wheat	kg	0.25	Own calculation
Ammonium sulphate	kg	2.24	[10]
Compressed CO_2	kg	0.70	[10]
Enzymes	kg	9.0	[17,18]
Transport, transoceanic tanker	tkm	0.01	[10]
Transport, transoceanic ship	tkm	0.01	[10]
Transport, lorry >32 ton, EURO5	tkm	0.08	[10]

GHG intensities of other materials, not mentioned in Table S.3, were obtained from the ecoinvent 3.2 database [10].

3.2 Emissions from land-use change

Table S.4 Emissions from land-use change [8,16,19,20].

Crop	Country	Conversion mechanism		Yield	Change in carbon stock
		from	to	kg/ha	t C/ha/a
Wheat	Germany	Set-aside land	Cropland	7900	-1.13
Soybean	Brazil	Scrubland	Cropland	2798	-3.80
Oil palm	Malaysia	Permanent Cropland	Plantation	24978	1.29
		Continental rainforest	Plantation		-6.70
	Indonesia	Insular rainforest	Plantation		-8.50

3.3 Sensitivity analysis

In the following section the effect of changes in several key parameters and the effect of different LUC assumptions is assessed (Table S.5). Changes in production modalities affect GHG savings estimated by RED methodology[4] and thereby alter the quantity of biofuel to be blended with fossil fuel as well as the amount of co-products resulting in a change in substitution mechanisms.

[4] The terminology „*GHG savings*“, here and hereafter, exclusively refers to the value calculated by RED methodology (Eq. 1) and does not present an occurring reduction in GHG emissions. In contrast, terms like "*decrease in GHG emission*" or "*increase in GHG emission*" refer to estimations of changes in emissions based on the consequential approach, thus respecting occurring changes in emission due to changes induced by the change in the system (i.e. introduction of 2G ethanol).

Table S.5 Assessed aspects in the sensitivity analysis

Section	GHG savings according to RED	GHG emissions based on consequential approach
3.3.1	Process heat demand	Process heat demand
3.3.2	Conversion efficiency	Conversion efficiency
3.3.3		GHG savings according to RED methodology
3.3.4		LUC emissions: wheat grains
3.3.5		Cultivation practice: soybean
		LUC emissions: soybean
3.3.6		LUC emissions: oil palm

3.3.1 Dependency of results on energy demand

The 2G process concepts modelled in this paper are not at full market maturity yet. Thus, process parameters of commercially competitive 2G facilities are largely unknown. Therefore, a change in heat demand is assessed to see its significance to overall results. The sensitivity analysis shows that the effect of a change in energy demand is low. The relative change in GHG savings remains below 10 % for all concepts if the energy demand changes by 10 %. The energy demand effects the consequential model by two aspects: (1) a change in GHG savings alters the quantity of fuel to be blended with fossil fuel to achieve legal targets, and (2) by altering the quantity of electricity provided as a co-product. The sensitivity analysis indicates that a change in heat demand does not affect results by a large extent (Figure S.4).

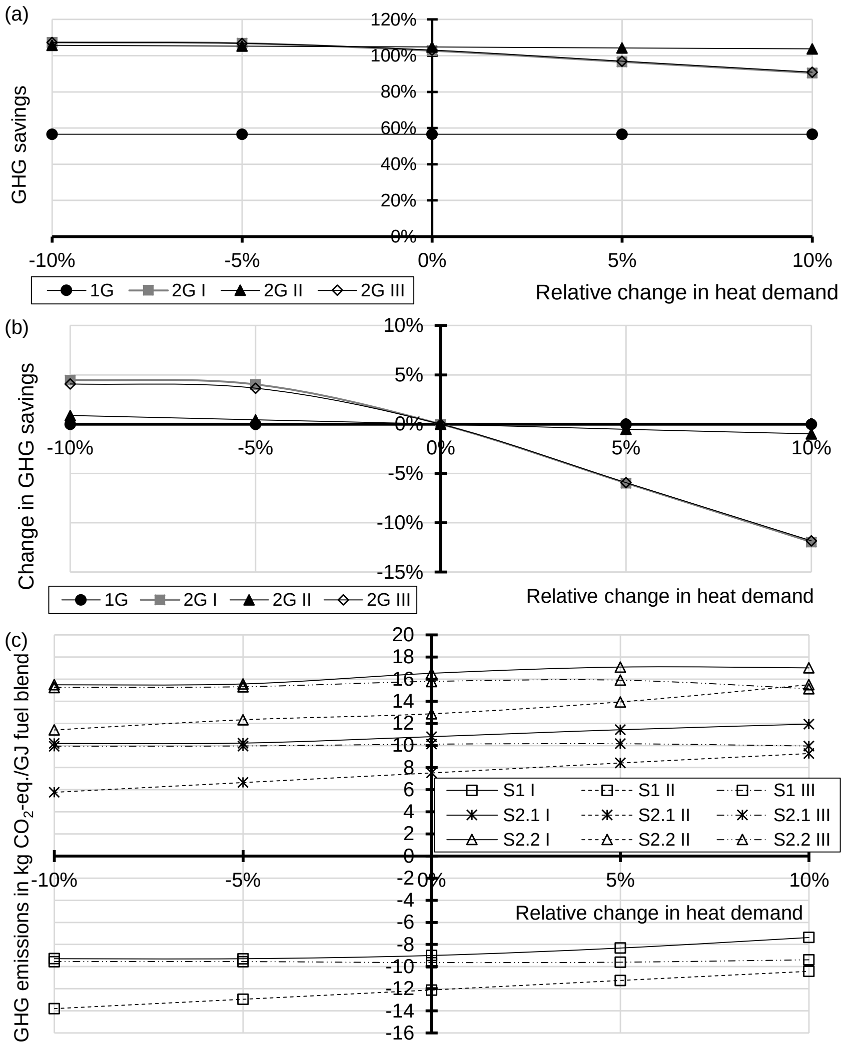


Figure S.4 Dependency of GHG savings and GHG emissions on a change in process heat demand: (a) absolute and (b) relative change in GHG savings according to RED methodology, and (c) change in GHG emissions due to a production of 1G and 2G ethanol and a shift from 1G to 2G ethanol production**.**

3.3.2 Dependency of results on conversion efficiency

The conversion efficiencies assumed in this paper are based on literature research and are thus subject to uncertainties. Again, a change in quantities affects the system by altering GHG savings and by changing the quantity of feed co-product (molasses) and the amount of electricity that is generated from solid residues. The sensitivity analysis shows that a change in conversion efficiency does not affect results to a large extent. A lower process efficiency results in more feedstock needed but at the same time, increases co-products, which lower the allocation factor of ethanol in the RED methodology and result in additional credits for feed and electricity in the consequential model.

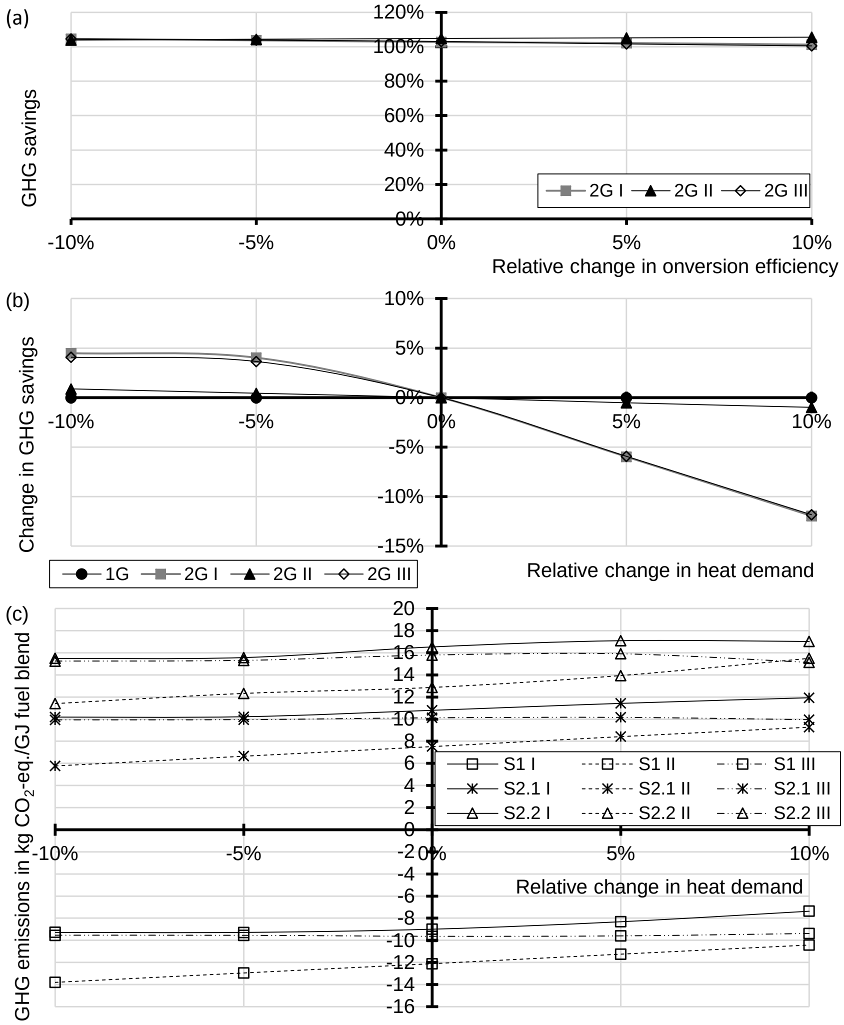


Figure S.5 Dependency of GHG savings and GHG emissions on a change in conversion efficiency: (a) absolute and (b) relative change in GHG savings according to RED methodology, and (c) change in GHG emissions due to a production of 1G and 2G ethanol and a shift from 1G to 2G ethanol production**.**

3.3.3 Dependency of results on GHG savings according to RED methodology

The quantity of fuel to be blended with fossil fuel is dependent on GHG savings according to the RED methodology. Figure S.6 shows the change in GHG emissions as a consequence of a change in GHG savings without affecting the quantity of co-products, e.g. by a change in emissions from feedstock cultivation. Results are most sensitive to changes in GHG savings of 1G ethanol, while GHG savings of other concepts remain fixed (case (c)): in scenario 1, the reduction of GHG emissions is reduced, while, in scenario 2.1 and 2.2, the increase in GHG emissions decreases. Thus, as higher the GHG savings according to RED methodology of 1G ethanol, and thereby, as closer the GHG savings of 1G and 2G concepts, the lower the change in emission. The same effect can be observed in case of a change in GHG savings of 2G concepts (case (b)).

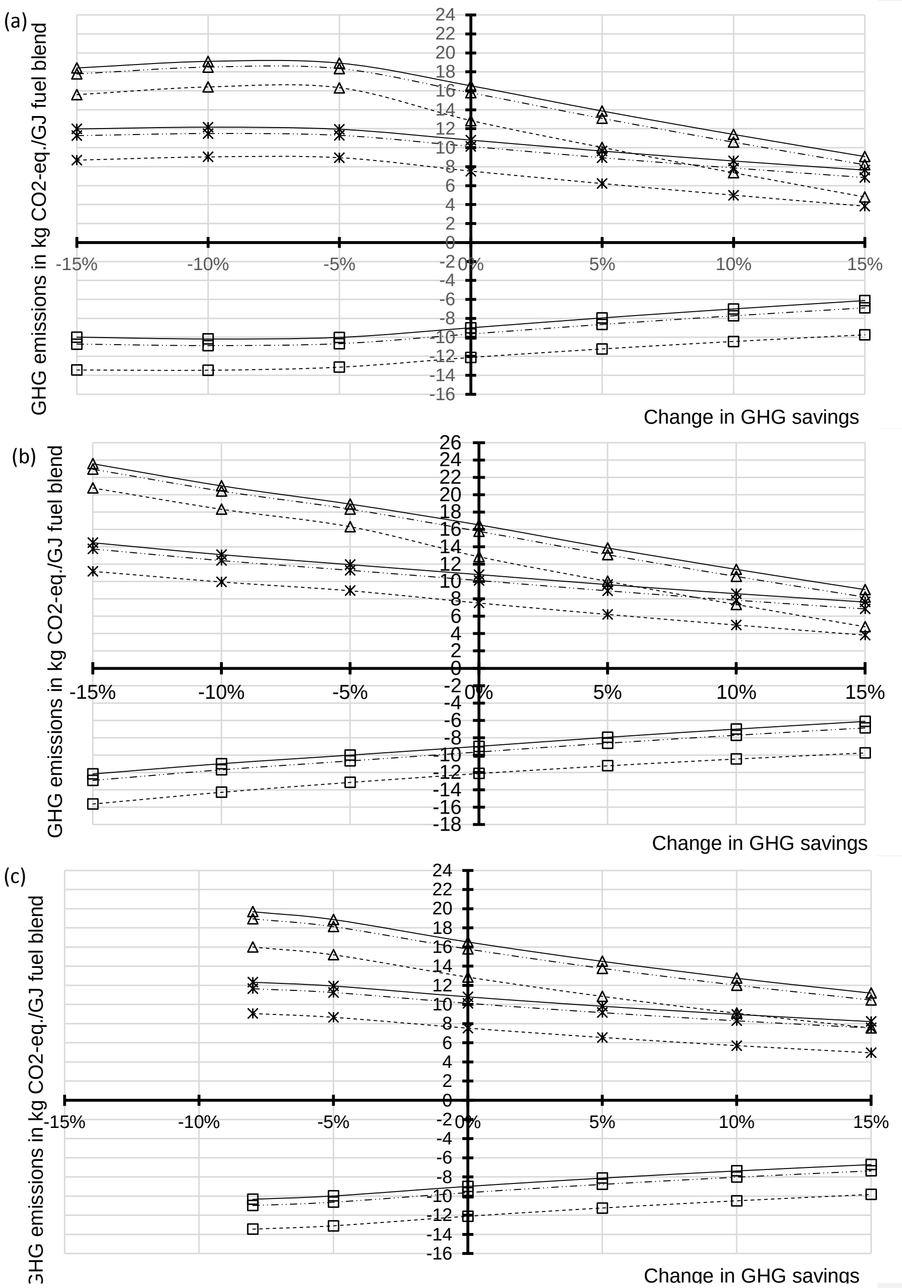


Figure S.6 Change in GHG emissions (consequential approach) in dependence of a change in GHG savings based in RED methodology (attributional approach): (a) GHG savings of 1G and all 2G concepts change, (b) 1G remains 58%, 2G concepts change, and (c) 2G concepts remain unchanged, 1G GHG savings change. Note: The minimum GHG saving requirement is 50 % as of 2020. Hence, 50% is the fixed minimum in case of (a) and (c) in case of 1G ethanol.

3.3.4 LUC emissions from wheat production

Results presented in Figure 6 (main text) refer to the change of agricultural land to fallow land as a consequence of wheat grains that become available. In Germany, agricultural land decreased by 0.47 million ha, while forest and settlement area, including infrastructure, increased by 0.28 and 0,32 million ha, respectively, between 2004 and 2014 [15, 17]. As an alternative to the presented LUC variant (conversion to fallow land), the conversion to forest (F_{LU} = 0.1, F_{MG}= 1, $C_{veg_{0-T}} = C_{veg_0} = 27\ t/ha$) is assessed [15]. In scenarios S2.1 and S2.2, it is therefore assumed that 46 % of unused cropland is converted to forest while 54 % are used for construction of buildings and infrastructure. In case land that becomes available eventually becomes a forest, the increase of GHG emissions from a shift from 1G to 2G ethanol will be lower (Figure S.7): the change ranges from 6 to 9 % of total emissions.

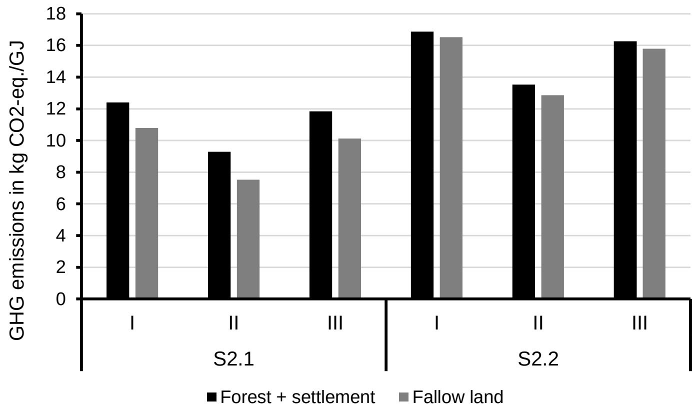


Figure S.7 GHG emissions due to the shift from 1G to 2G ethanol in dependence of LUC assumptions for wheat grains.

3.3.5 Soybean cultivation: Cultivation practice, location and related LUC emissions

Soybean cultivation and related LUC are the largest contributor to an increase in emissions due to a shift from 1G to 2G ethanol (scenarios S2.1 and S2.2, Figure 7 (main text). Figure S.8 shows emissions per GJ fuel blend for 2G concept I with respect to changes in production modalities and LUC. The soybean yield (2978 kg/ha) has been adapted based on [18]: 3332 and 3428 kg/ha in case of reduced and no tillage, respectively. The sensitivity analysis reveals that for most biomes, emissions changes will remain positive in case of a shift from 1G to 2G ethanol. Only if no LUC occurs or if soy is cultivated on severely degraded savanna, emissions will be reduced by a shift from 1G to 2G ethanol. The effect of cultivation practice is in most cases negligible in comparison to total emissions or effects of changes in biomes in which LUC emissions occur.

Table S.6 Parameters for sensitivity analysis of cultivation practice, location of cultivation and LUC as well as different LUC scenarios [15, 18]. Abbr.: BR – Brazil, I – improved management, LAC – low activity clay, M – moderately degraded, NT – no tillage, RT – reduced tillage, S – severely degraded, T – tillage; parameters as defined in Eq. 9 and 10. The reference assumptions are marked in bold.

Location	Climate	Soil	Land use		SOC, ref [t C]	F,LU	F, MG	F, I	C,veg [t C]	C total [t/ha/20a]
BR, Central West	Tropical moist	LAC	Soy plantation	NT	47	0.48	1.22	1	0	28
				RT	47	0.48	1.15	1	0	26
				T	**47**	**0.48**	**1**	**1**	**0**	**23**
BR, South	Warm temperate	LAC		NT	63	0.69	1.15	1	0	50
				RT	63	0.69	1.08	1	0	47
				T	63	0.69	1	1	0	43
BR, Central West	Tropical moist	LAC	Savanna	I	47	1	1.17	1.11	53	114
				M	**47**	**1**	**0.97**	**1**	**53**	**99**
				S	47	1	0.7	1	53	86
			Tropical Rainforest		47	1			198	245
			Forest plantation		47	1	1	1	58	105
			Perennial crop	NT	47	1	1.22	1	14.4	72
				RT	47	1	1.15	1	14.4	68
				T	47	1	1	1	14.4	61
BR, South	Warm temperate	LAC	Forest plantation		63	1	1	1	31	94
			Perennial crop	NT	63	1	1.15	1	43.2	116
				RT	63	1	1.08	1	43.2	111
				T	63	1	1	1	43.2	106
			Grassland	I	63	1	1.14	1.11	6.8	87
				M	63	1	0.95	1	6.8	67
				S	63	1	0.7	1	6.8	51

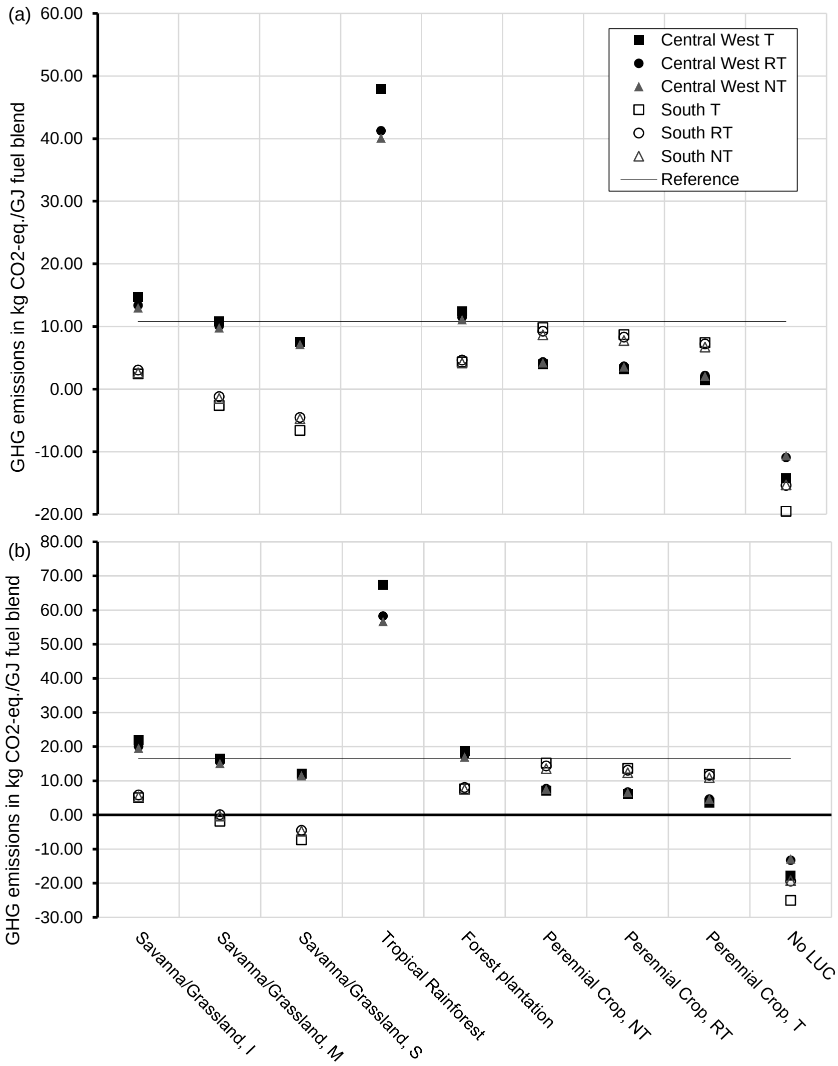


Figure S.8 GHG emissions per GJ fuel blend of 2G concept I, scenarios S2.1 (a) and S2.2 (b), in dependence of cultivation practice of soybeans (tillage (T), reduced tillage (RT), no tillage (NT)), cultivation location (Central-West and Southern Brazil) and the biome where LUC occurs. The reference line presents the value without any changes for sensitivity analysis. Abbr.: I – improved management, M – moderately degraded, NT – no tillage, RT – reduced tillage, S – severely degraded, T – tillage.

3.3.6 LUC emissions from oil palm cultivation

As a consequence of the shift from 1G to 2G ethanol, DDGS is not supplied anymore. DDGS is replaced by soybean meal which results in a provision of vegetable oil. This oil reduced demand for other vegetable oil (see section 2.4). Thus, the shift triggers a reduction in demand for palm oil. The effect of a change in biome where LUC of oil palm cultivation occurs reveals that in most cases, GHG emissions in both scenarios increase when the biome changes (Figure S.9). This is due to the fact that less carbon is stored in most biomes listed in Table S.6, e.g. perennial plantations, compared to native rainforest (as assumed in the analysis). Likewise, the emission increase that results from a shift from 1G to 2G ethanol (scenario 2) is lower if palm oil is substituted that originates from biomes where formerly large quantities of carbon where stored, e.g. peat. Regardless of the biome, the shift from 1 to 2G ethanol results in an increase in emissions.

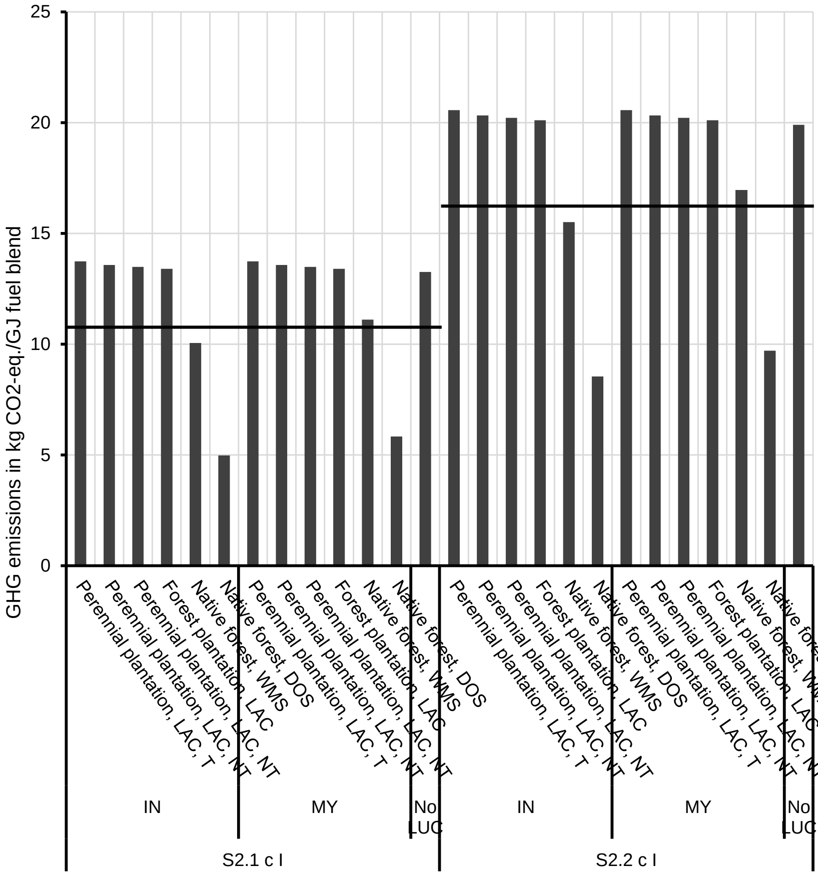


Figure S.9 GHG emissions per GJ fuel blend of concept I, scenarios 2.1 and 2.2, in dependence of the biome where LUC of palm oil cultivation occurs assuming a 100% provision from the respective biome and location. The reference line presents the value without any changes for sensitivity analysis. Abbr.: DOS – drained organic soil (peat), IN – Indonesia, LAC – low activity clay soil, LUC – land-use change, MY – Malaysia, NT – no tillage, RT – reduced tillage, T – tillage, WMS – Wetland mineral soil.

Table S.7 Parameters for sensitivity analysis of location of cultivation and related LUC emissions of oil palm cultivation **[15, 19]**; DOS – drained organic soil (peat), IN – Indonesia, LAC – low activity clay soil, LUC – land-use change, MY – Malaysia, NT – no tillage, RT – reduced tillage, T – tillage, WMS – Wetland mineral soil

				SOC, ref	F,LU	F, MG	F, I	C,veg	On-site CO_2	Off-site CO_2	CH_4	N_2O	C total
Location		Land use		[t/ha]				[t/ha]	[t C/(ha a)]	[t C/(ha a)]	[t CO_2-eq./(ha a)]		[t/ha]
IN	LAC	Perennial plantation	T	60	1	1	1	34.3					94
			RT	60	1	1.15	1	34.3					103
			NT	60	1	1.22	1	34.3					108
		Forest plantation		60	0.8	1	1	64					112
	WMS	Oil palm plantation		49	1	1	1	60					109
		Native forest		49	1			230					279
	DOS	Oil palm plantation						60	11.0	0.8	1.1	0.6	-210
MY	LAC	Perennial plantation	T	60	1	1	1	34.3					94
			RT	60	1	1.15	1	34.3					103
	LAC		NT	60	1	1.22	1	34.3					108
		Forest plantation		60	0.8	1	1	64					112
	WMS	Oil palm plantation		49	1	1	1	60					109
		Native forest		49	1	0	0	185					234
	DOS	Oil palm plantation			1	1	1	60	11.0	0.8	1.1	0.6	-210

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