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Economic and agronomic impact assessment of wheat straw based alkyl polyglucoside produced using green chemical approaches

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A B S T R A C T

Results from a previous environmental impact assessment highlight the potential for the proposed process, that converts low-value agricultural residue (wheat straw) into a high-value biosurfactant, to result in significant (>75%) GHG savings, relative to the commercial candidate derived from palm kernel and wheat grain. This was achieved via the use of low-energy techniques like supercritical CO_2 extraction, low-temperature microwave and in-situ fractionation of platform chemicals. Despite the environmental benefits, process commercialization relies on the economic feasibility of the production. Adopting a ‘cradle-to-gate’ life cycle costing approach, this paper has quantified the economic feasibility and resource efficiency characteristics of producing wheat-straw based APG, via the previously suggested green low-waste generating processes. Here, we undertook economic analysis of a wheat straw-derived APG production pathway, in comparison to palm-kernel and wheat-grain APG. Total processing costs were determined to range between $0.92- $1.87 per kg of wheat straw-APG demonstrating relatively better output service quality and energy efficiency, while conventional APG costs $1.95- $2.87 per kg, highlighting the significant potential of the residue-derived pathway to be scaled to commercial-level. In addition, a semi-quantitative assessment of the demand-based implications of adopting and scaling-up the green process, in the current context and practices of wheat cultivation was also undertaken. Potential agronomic impact that might be result from such scale-up scenarios, focusing on the effect of conventional residue incorporation practiced by farmers was assessed in detail to encourage farmers opt for informed choices and also to encourage both environmentally and economically sustainable systems-thinking.

1. Introduction

An increasing awareness of the negative environmental impact of petroleum based products and, the overall performance benefits of bio-surfactants, have encouraged market demand for ‘bio-derived surfactants’, especially for their application in high value products (mainly personal care products and cosmetics (Hexa Research, 2016; Pantellic, 2014a; Saharan et al., 2011) which is evident from Fig. 1.

Alkyl polyglucosides (APG), introduced between 1980 and 1990, have their hydrophobic and hydrophilic groups sourced from plant derived fatty alcohol and sugars. World-wide consumption of surfactants was reported to be 9300 kT in 2000 and this market is projected to reach 24,000 kT by 2020. With the global biosurfactant market reaching 350 kT in 2015, global APG production alone reached 90 kT in 2015 and Europe was the largest producer and consumer generating associated revenue of £700 m (Transparency Market Research, 2015). Europe is currently the largest producer and consumer of alkyl polyglucoside owing to the product's relatively low (ecological and human) toxicity coupled with stringent environmental regulations from regional enforcement authorities such as the European Environmental Agency (EEA), European Chemicals Agency (ECHA) and REACH (Registration, Evaluation, Authorisation and restriction of Chemicals). However, at an annual APG growth rate of 5.5% in Asia pacific (China and India), it is expected to overtake Europe's production by 2023 (130 kT annual

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production projection and revenues of £580 m) (GM Insights, 2016).

The techno-economic evaluation of such an economically significant commodity has been undertaken only by a handful of studies (Adlercreutz et al., 2010; Kosaric and Vardar-Sukan, 2015)). Since there is constant evolution within the surfactant industry and better surfactants are created with time, technology and innovation, studies are either class-specific or product specific in the nature of their assessment. The focus lies solely on the production technology and seldom from a supply-chain perspective. The main cost-contributing element of synthesis of any bio-based product is the choice of feedstock. There is an increase in the attention to the use of chemical feedstock from waste and residues that are generated from other industries, particularly as these have the potential to displace fossil derived products without the need for additional procurement, production systems or land use (Saharan et al., 2011). Some life cycle studies have investigated the potential of a range of sugar and lipid-enriched industrial wastes/residues (Saharan et al., 2011; Costa et al., 2009; Adlercreutz et al., 2010) including whey from dairy industry, molasses from distillery, animal fat and tallow for the production of biosurfactant. However, these production methods employ environmentally non-benign solvents and expensive catalysts, questioning the sustainability aspect of such “bio-based” products.

The aim of the study undertaken, and presented in this paper, is to quantify the potential costs associated to producing alkyl polyglucosides by the cascading use of relatively low-value agricultural residue employing optimised green chemical approaches, as opposed to the conventional approach of utilising first-generation sources such as palm-kernel and wheat grain. In addition, appropriate resource efficiency indicators adopted from bioenergy related studies and modified for application to biomaterials evaluation have also been employed.

Quantified inputs (material and energy) and outputs (products, by-products, emission and wastes) of the WS-APG processes have been obtained from the research team that conceived the process (Fan and Budarin, 2016; Budarin et al., 2009; Priecel and Lopez-Sanchez, 2015) and for the baseline process, an earlier published literature was consulted (Guilbot et al., 2013).The life cycle inventory for this study has been provided in the supplementary information.

For brevity, APG synthesised from wheat straw will be referred to as WS-APG and that synthesised from palm kernel and wheat grain will be referred to as PW-APG. The “cradle-gate” life processes associated to the production of APG from wheat straw and the baseline feedstocks, wheat grain and palm kernel have been presented in Figs. 2 and 3.

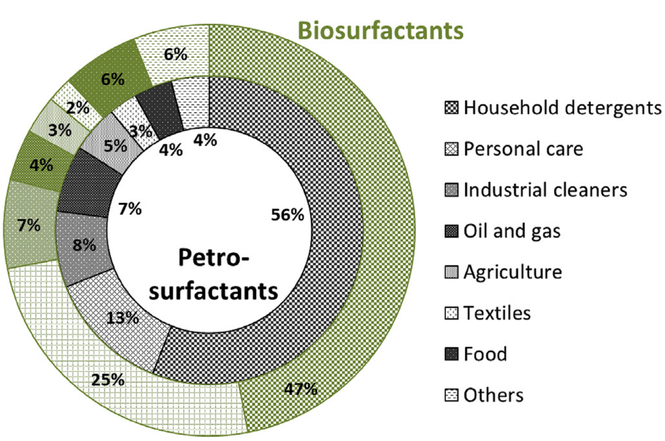

Fig. 1. Market demand for biosurfactant (Pantellic, 2014b).

In order to demonstrate and justify the ‘sustainability’ of any greener production alternatives, the environmental impact, economic feasibility capturing the overall indirect impacts should be assessed. Therefore, a semi-quantitative agronomic study encompassing a hypothetical scenario of industrial scale up of the production process was also undertaken. Scenarios related to this potential scale-up of APG production and the impacts of resulting economic-environmental trade-off on agricultural soil have been assessed.

Unlike environmental LCA which is standardised under ISO 14040, LCC methods are not captured though ISO standards or equivalent guidelines. Therefore, LCC are undertaken based on expert knowledge and industrial best practices. The two types of costs considered in LCC are fixed and operating costs. Of the two, the operating costs are generally variable and influenced by product. The aim of this exploratory analysis is to quantify the economic viability of producing a high value biosurfactant from a low-cost feedstock at a pilot scale, emphasising costs associated to material use, energy consumption and labour, also comparing the productivity of two different biomass. As a result, unlike conventional LCC, this study does not involve a ‘break-even’ analysis and the economic impact analysis is based on variable costs alone. Further explanations of this assumption have been presented under appropriate segments in the “methods” section.

2. Methodology

2.1. Life cycle costing

Conventional LCC requires the quantification of fixed costs and operating costs associated with the installation, operation, maintenance, insurance of a facility and production of a given product, in addition to the value of the investment at the end of the facility's useful life. Due to this analysis being exploratory in nature, with an aim to quantify only the production and labour costs in a pilot scale facility, this paper encompasses purely the operating cost of the proposed process for WS-APG production, excluding any fixed costs, maintenance or any other expenses associated with the installation of the facility. Due to the use of green approaches and specialist equipment, projection of fixed and maintenance costs at such an early stage of process commercialisation is likely to introduce considerable uncertainties leading to inaccurate results. Upon quantification of the costs associated with the production of APG from wheat straw (WS-APG), the outcome is compared to the process economics of the baseline case study, where the APG is conventionally synthesised from palm kernel and wheat grain (PW-APG). Due to the lack of an appropriate techno-economic investigation of the commercial baseline case study, this paper takes on to predict the processing costs (as $/kg APG) for the baseline candidate, PW-APG, based on the data for process material and energy needs presented in the previously published literature (Guilbot et al., 2013). For information, it is essential to note that currently PW-APG, in the commercial market, costs anywhere between $1.60-$3.20/kg (Alibaba.com, 2018).

The production cost is predicted through integration of the unit prices corresponding to the quantified inputs and outputs (particularly processed and unprocessed wastes) for both the target analysis and baseline scenario. This approach (also called as normalisation) refers to the process of combining the methodology and data used for environmental life cycle assessment with life cycle costing which besides overcoming the limitations of independent economic evaluation (e.g. difficulties with model development/boundary expansion, time intensive and human error with data inputs) also enables a consistent and parallel evaluation of sustainability, within the user-defined system boundary.

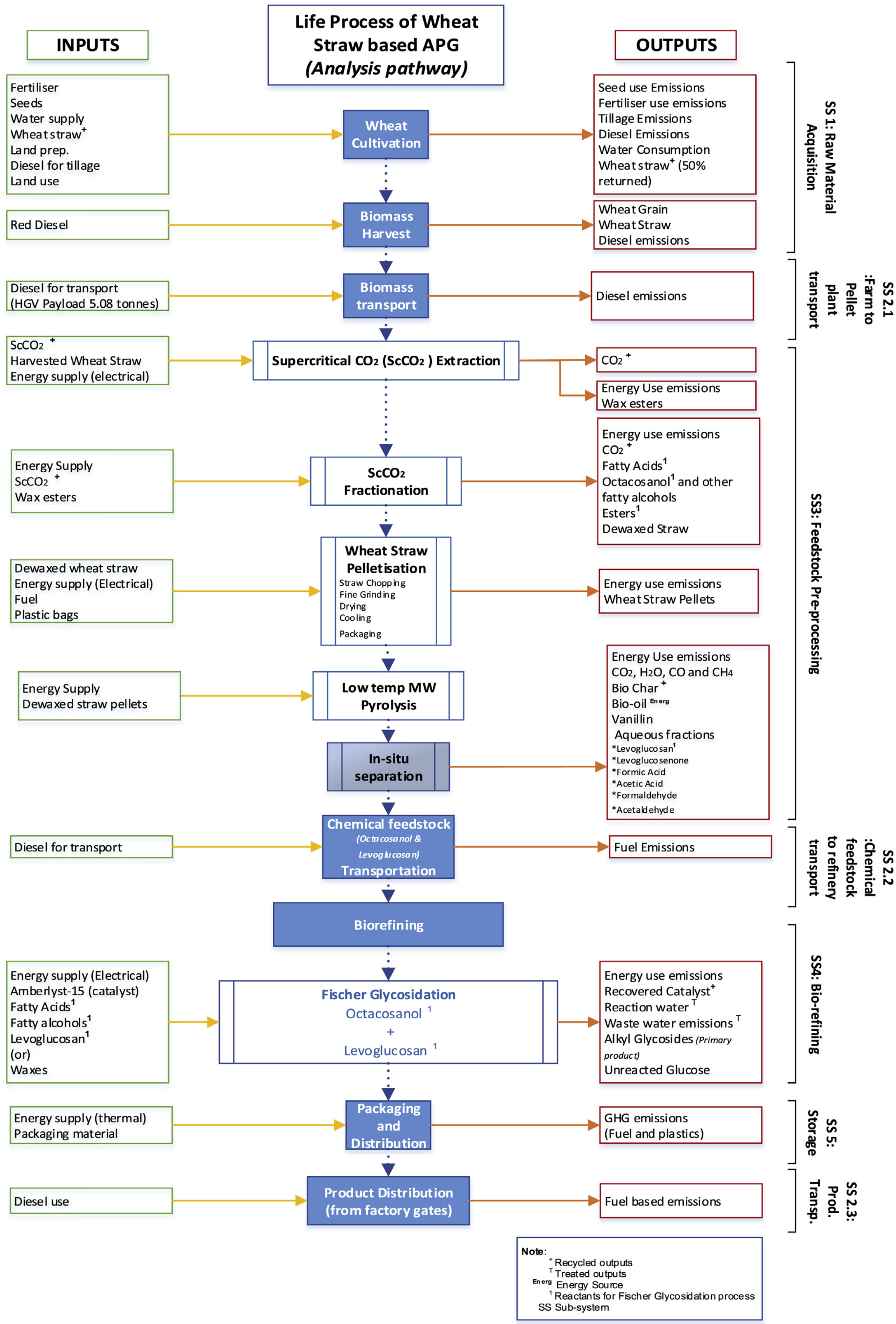

Fig. 2. Cradle-gate life cycle stages for WS-APG production (source: Lokesh et al., 2017).

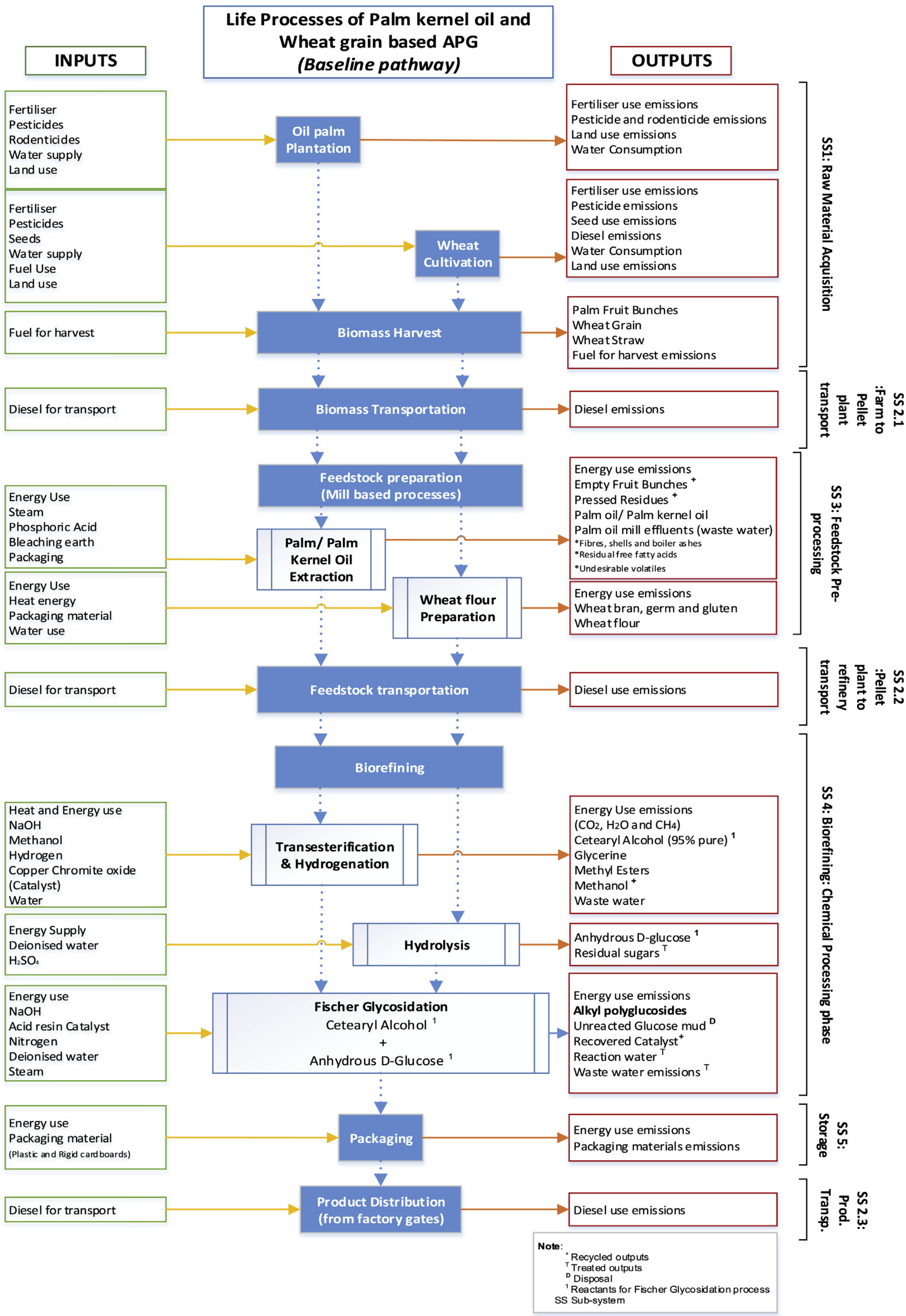

Fig. 3. Cradle-gate life cycle stages for Palm kernel and wheat grain based APG (PW-APG) production (Data source:(Guilbot et al., 2013)).

The methodology associated to the stage-level material and energy cost calculation for both the analysis (WS-APG) and baseline (PW-APG) pathways, appropriate assumptions on the cost calculation at local currency and conversion to standard ($) currency have all been presented in the Appendix A.

2.1.1. Biomass cultivation and harvest

With any conventional life cycle study, the spatial and temporal boundaries of this analysis had to be established. The wheat-straw based APG is assumed to be locally sourced with the pre-treatment and biorefinery facilities located in the UK. In the case of our baseline candidate palm-kernel and wheat based APG, palm kernels were assumed (Guilbot et al., 2013) to be sourced from Indonesia and upon refining, the chemical feedstock (palm kernel oil) was transported to Europe by sea (Guilbot et al., 2013). The pre-treatment and biorefinery facilities, in the baseline studies, was suggested to be located in Europe.

To ensure consistency, the pre-determined system boundary (“cradle-to-factory gate”) from the previous environmental impact assessment (Lokesh et al., 2017) was adopted for the economic analysis. The raw material for the synthesis of wheat straw-APG was acquired from wheat cultivation and harvest, the starting point of this LCC. This study assumes that the proposed process adds value to the agricultural residue, as a result of which, the cost of wheat cultivation is also allocated based on %mass of wheat straw and wheat grain generated from feedstock cultivation. For information, the prices for the commodities that feed into biomass cultivation phase for both WS-APG and PW-APG have been summarized and listed in the Appendix Table B.1.

Upon harvest of the wheat grain, only 50% of wheat straw is harvested leaving the other 50% to be chopped and spread for recirculation into soil. This is an important agronomic step to ensure the return of the organic nutrient content back to the soil and its subsequent conditioning of the soil and other soil health benefits. The harvested straw is baled, carted out of the farm and sold. In 2017 (time of analysis), wheat straw was sold at a price of $50/ton (Agriculture and Horticulture Development Board, 2018a).

2.1.2. Transportation stage

WS-APG: In the analysis case the feedstock from each of facilities is assumed to be transported to their destination via road (Guilbot et al., 2013). Further information on these assumptions have been detailed in the Appendix section A.2. The harvested wheat straw is assumed to be transported to the pre-treatment facility located at a distance of 150 km using a low-sulphur diesel truck.

PW-APG: For the baseline case, the assumptions drawn from the baseline case study (Guilbot et al., 2013) is presented in supporting information section 1.1.2 [Note: the oil palm and wheat croplands are based in Indonesia and France respectively, as a result of which region-specific fuel prices will be used]. The costs incurred by transportation of feedstock and products are calculated using the equation below

$$Transp._{GHG_D} = \frac{\sum_{i=1}^{n} Fuel\ use_{1-n} \times Costs_{fuel\ cons.}}{Total\ mass\ of\ APG\ .ha^{-1}} \quad (1)$$

where, n	= *number of commodity transfers*
$Fuel\ use_{1-n}$	= *fuel (e.g. diesel or HFO) consumed between the destinations (l)*
$Costs_{fuel\ cons.}$	= *unit price of fuel type ($/l)*

The fuel prices for different fuel types, adopted for this study are shown in the Appendix section table B.1.

2.1.3. Pre-processing stage

Baled wheat straw (with the moisture content of avg. 13.5%), is transported to the pre-treatment plant where it is ‘blow-dried’. Dried wheat straw is then milled to provide a greater access to the straw surface for the supercritical solvents to act on and extract waxes off the surface in the upcoming wax extraction stage. The extracted wax amounts to roughly 1–2% by mass of the total wheat straw fed into the process. The advantages of the supercritical solvent extraction stage is two-fold: the wax ester is the source of fatty alcohol required to contribute the hydrophobic component to the surfactant molecule; and removal of waxes facilitate better access to cellulosic components for the upcoming low-temperature microwave pyrolysis stage. The fatty alcohol that renders the hydrophobic building blocks to the APG molecule is n-octacosanol, a straight chain 28-carbon organic fatty alcohol which is isolated from the waxy mixture (waxes, esters and fatty acids) through supercritical CO_2 fractionation (Lokesh et al., 2017; Mašek et al., 2013).

The dewaxed wheat straw was then pelletized by pressuring it through a heated “die”. The -pelleted wheat straw was then subjected to low-temperature microwave pyrolysis at 130–150 °C for 7–8 min, over the period of which the different aqueous and organic fractions of solid, liquid and gaseous products and by-products were generated. The quantified outputs of this pre-treatment stage has been presented in the Fig. 4.

These products were isolated via in-situ separation. According to the Budarin and Fan (Budarin et al., 2009; Fan and Budarin, 2016), 1 kg of dried pelleted wheat straw provided 30 g of levoglucosan, a 6-carbon organic sugar molecule which contributes the hydrophilic component to the surfactant molecule (Budarin et al., 2009; Lokesh et al., 2017). More details on the inputs and outputs of this process have been presented in the Fig. 4. The unit prices of commodities that found application in the pre-processing stages of both the WS-APG and PW-APG have been presented in the appendix Table C.1 of the supplementary information.

2.1.4. Biorefinery and packaging stages

Fischer glycosidation was the chosen pathway for WS-APG production where n-octacosanol and anhydrous sugars (levoglucosan), acquired from the pre-processing phase, were reacted with each other in the presence of an acid catalyst, sulphuric acid. In addition to the synthesis of the desired APG, other by-products such as anomers, isomers and acyclic compounds are likely to be formed. Unreacted sugars resulting from this process were disposed through incineration. The isolated APG was then stabilised through the use of de-ionised water and ethyl acetate, which was then recovered for re-used. The material/energy specification and the process description for the biorefinery, packaging and distribution of WS-APG and PW-APG have been described in detail in the environmental analysis in the supporting information. However, the schematic presented in Fig. 4, provides information on the material and energy inputs/outputs across the various stages of WS-APG production. The life cycle inventory for the baseline case study has been published by the authors of the previously published paper (Guilbot et al., 2013).

2.2. Measuring resource efficiency

The proposed process of the production of WS-APG which utilises and agricultural residue with the added benefit of responsible soil-organic matter management, has the potential to adhere to the

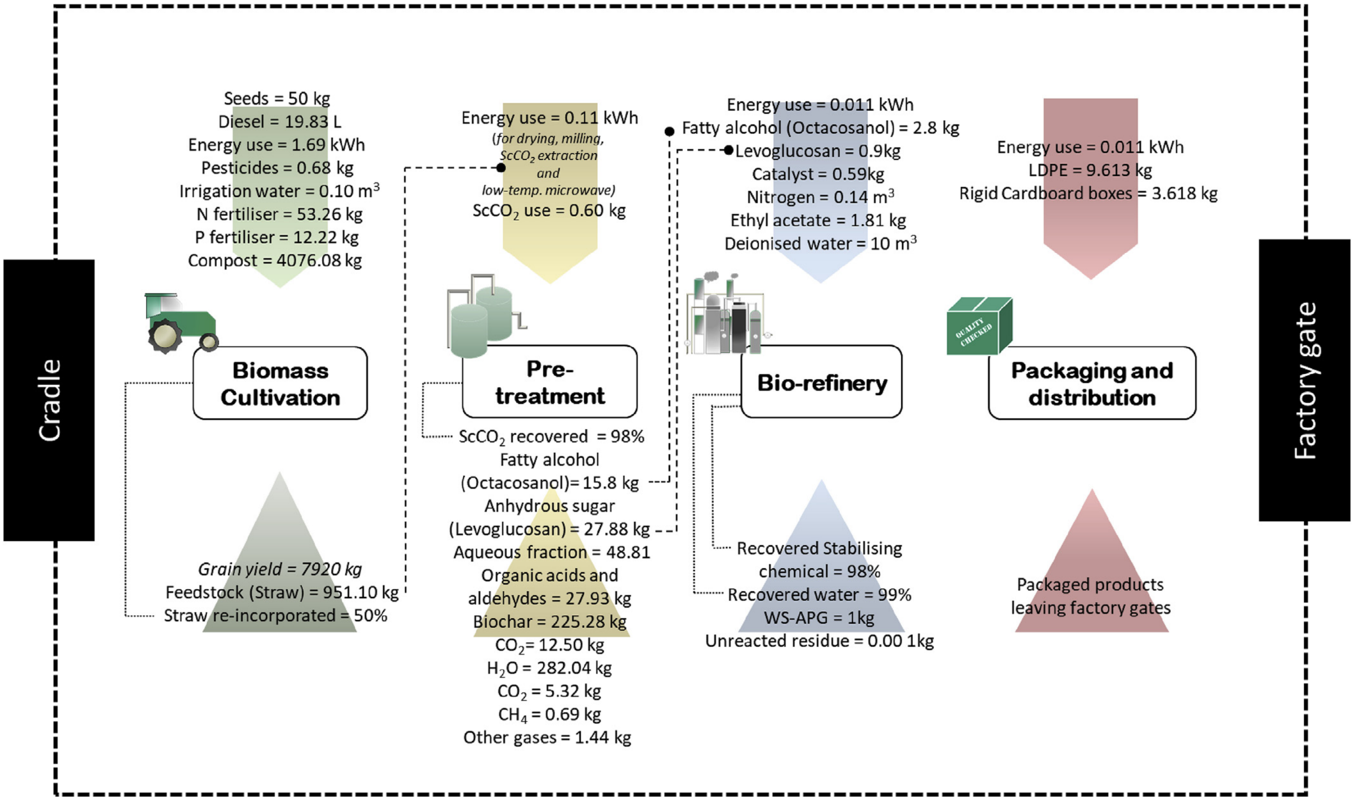

Fig. 4. Life cycle inventory for the production of 1 kg of wheat straw based APG.

principles of circular economy. Circular economy, though appearing to be quite complex in our current infrastructure, can satisfy our sustainability goals. In general, a fully functional, circular, bio-based value chain has the potential to contribute directly to atleast 11 of the 17 Sustainable Development Goals (UN SDGs), addressing all the three pillars: environmental performance, economic feasibility and social impact. In an attempt to identify the linkages between the proposed value chain and highlight their circularity characteristics, this study has adopted some unconventional semi-quantitative "resource efficiency" metrics, in addition to the aforementioned "life cycle costing" approach. Technically, resource efficiency can be interpreted to the efficient utilisation of the material and energy to meet our needs. Resource efficiency is one the main strategies in achieving a fully-functional circular economy and according to the European Environmental Agency (2013), the aim of circular economy is to decouple economic growth from resource utilisation. Some of the various metrics adopted for this study include functionality (output service quality) and energy efficiency.

Output service quality: Output service quality is measured as the difference in the economic value of the process outputs (products and by-products) relative to that of the process inputs, per dry tonne of biomass (a means of quantifying the value-added to the raw materials). This method provides a better insight by measuring the quality of service delivered by the value-added product in addition to demonstrating the effectiveness of the "value-addition" process. This approach was conventionally applied to highlight the energy output quality of bioenergy, to measure the energy output of the product in relation to the energy fed into the product. However, this valuable indicator has been adapted to this study to demonstrate the economic potential of a given product and co-products more than the conventional energy generation. This parameter measured as 'net $ output per dry tonne of biomass' input, was adopted from the methodology employed by Pelkmans et al. (2014) and may be expressed as follows

$$\textit{Output service quality} = \frac{\sum_{i=1}^{n}[(\boldsymbol{M}_{ou} \times \boldsymbol{p}_{\boldsymbol{i}}) + (\boldsymbol{E}_{\boldsymbol{ou}} \times \boldsymbol{p}_{\boldsymbol{i}})] - \sum_{j=1}^{n}[(\boldsymbol{M}_{in} \times \boldsymbol{p}_{j}) + (\boldsymbol{E}_{\boldsymbol{in}} \times \boldsymbol{p}_{j})]}{\textit{per dry kg of biomass}} \tag{2}$$

where,

- M_{in} = *Quantified material input in a given life stage (kg or m³)*
- M_{ou} = *Quantified material outputs in a given life stage (kg or m³)*
- p = *relevant unit prices (\$/kg or m³ of the material used)*
- E_{in} = *Quntified energy input in a given life stage (MJ or kWh)*
- E_{ou} = *Quntified energy output in a given life stage (MJ or kWh)*
- $i(j)$ = *"1 to n" refers to the approapriate material/energy inputs and outputs of the production phase*

Energy efficiency: In addition to decoupling economic growth from resource utilisation, the ultimate goal of a full-fledged establishment of circular economy is to “wean-off” our dependence on fossil-based resources. The suggested parameter directly connects to the utilisation of fossil-derived energy from “cradle-gate” production of the WS-APG, the economic value of which is measured and compared with that of the conventional candidate, PW-APG. This parameter is expressed as “net $ MJ input per kg of products and by-products produced” which can be calculated using the methods presented below.

$$\textit{Energy efficiency} \quad = \frac{\sum_{i=1}^{n}\left[(\boldsymbol{E_{inp}}) - (\boldsymbol{Int_{inp}})\right] \times \boldsymbol{p}_i}{M_{prod} + M_{BProd}} \tag{3}$$

where,

$M_{Prod, Bprod}$	= *Mass of products and byproducts generated from the process (kg)*
E_{inp}	= *Quantified energy fed into a given life stage (MJ)*
Int_{inp}	= *Quantified internally derived energy that was re-used into a process (MJ)*
P	= *relevant unit prices ($/MJ)*
i	= *“1 to n” refers to the different value-chain stages from whcih the energy consumption is accounted*

2.3. Calculation of labour costs

According to the baseline study, the international supply chain for PW-APG spans from Indonesia to Europe (Guilbot et al., 2013). Therefore, the influence of geographic location on the labour costs, in addition to the annual regional inflation rates must also be taken into account. The labour costs associated with each of the life cycle stages is calculated as $/kg of APG based on available literature. Labour costs adopted from earlier literature have been corrected to current scenario applying appropriate regional inflation rates. Further assumptions on labour costs calculation have been presented in Table 1 and in the Appendix in section E.

2.4. Sensitivity study

From conventional wisdom within life cycle studies, the biggest cost contributor in the life cycle costing of bio-based projects tend to be the feedstock generation stage (biomass cultivation in this stage). Considering this, the costs associated with biomass cultivation (BC costs) can be subjected to an argument between three scenarios, which entail mass or economic based allocation of overall costs calculated. A description of these three scenarios have been presented below.

2.4.1. Scenario 1: mass based allocation (baseline)

Biomass cultivation costs are partitioned between the wheat grain and wheat straw based on % mass (per ha) since this study is devoted to adding economic value to the wheat straw. Additionally, this feedstock is economically valuable finding application in a range of other sectors (soil recirculation, animal husbandry, electricity generation and horticulture). This assumption has been chosen as the default scenario for the core economic impact assessment.

2.4.2. Scenario 2: wheat straw as a low value “residue”

Biomass cultivation costs are solely allocated to the wheat grain when wheat crop is assumed to be solely cultivated for wheat grain and wheat straw (which is a residual by-product of this cultivation procedure) has been used to produce APG.

2.4.3. Scenario 3: economic significant commodity

Biomass cultivation costs partitioned between wheat grain and wheat straw based on their economic significance [Note: Wheat grain and wheat straw cost $230.66 and $50 per ton, respectively as of Nov 2017.

2.5. Agronomic analysis

To assess the economic feasibility of the process (which is undertaken assuming ‘pilot’ conditions rather than full-optimisation) the LCC assesses the cost of producing WS-APG from wheat straw obtained from a hectare of land, in line with the previous environmental assessment (Lokesh et al., 2017; Guilbot et al., 2013) However, the establishment of a commercial scale production would effectively require a continuous supply of feedstock and, therefore, an evaluation of the socio-economic impacts of such a scenario on the wheat farming community (as feedstock provider) which currently adopts a practice of straw incorporation into soil, has been undertaken. The significance of wheat straw incorporation to field productivity and the added benefits of high-quality biochar (a by-product of the microwave pyrolysis phase) incorporation via reduced demand for fertiliser application rates can be found from previously published literature ((Brennan et al., 2014; Karer et al., 2013; Sadeghi and Jafar Bahrani, 2009; Shindo and Nishio, 2011; Wei et al., 2015; Zhang et al., 2014)

Winter wheat is a major cultivated-crop in the UK that reached an avg. annual production rate of 14.5 million tonnes between 2011 and 2017 (National Statistics-UK, 2017). With wheat harvest in the UK, averaging an 8800 kg/ha, in 2017, wheat straw harvest can be safely assumed to have reached 4480 kg/ha. [Note: Wheat straw production predicted by applying a harvest index of roughly 50% (in the UK) to wheat grain production] (ADHB Cereal and Oilseeds: Wheat, 2016). To account for losses during storage (i.e. from

Table 1
Labour costs ($/kg) calculated for WS-APG and PW-APG synthesis.

Life Cycle Stages	Assigned Labour costs ($/kg)			Sources
	WS-APG	PW-APG		
	Wheat straw	Wheat grain	Palm Kernel	
Biomass Cultivation	0.01	0.02	0.03	(Farmers Weekly, 2013)
Pre-processing	0.20	0.00	0.04	(Attard et al., 2015; Finlayson, 2012; Nilsson et al., 2011)
Refining, Package and storage	0.13	–	0.13	(Li and Mupondwa, 2012)
Transportation costs	0.01	0.04	0.03	(Agriculture and Horticulture Development Board, 2018b)
Total	**0.35**	**0.24**	**-**	

Note:
For information acquired from the references before 2017, appropriate regional inflation rates have been applied to the labour costs and calculated.
* Refining and packaging labour costs for WS-APG were assumed to be similar to that of PW-APG due to the similar set of processes.

microbial/weed contamination and rotting due to excess moisture during the winter season which in this study is considered a worst case scenario), this study assumes straw biomass losses of upto 950kg/ha (based on data from (Agriculture and Horticulture Development Board, 2016a; BIOCOmmodity REfinery, 2012), leaving a net mass of about 3530 kg/ha. Scaling up this yield of wheat straw to annual UK production amounts to 13.3 million tonnes of which 6.65 million tonnes is set aside for bale and sale. Wheat straw yield, for this study, has been calculated from the fraction that is harvested in Yorkshire and Humber. The remaining fraction is, by current practice, returned back to the agricultural soil for nutrient cycling and maintenance of soil organic matter. According to the (Agriculture and Horticulture Development Board, 2018a) 6.65 million tonnes of wheat straw is assumed to find application in various sectors including

- Animal husbandry – 47.3%
- Horticulture – 3.63%
- Energy – 2.45%
- Export – 0.65%

[**Note**: roughly 40% of the feedstock already finds application in other sectors while the other 46% (remaining) is destined for soil re-incorporation.]

An agronomic study was undertaken as a part of this economic impact evaluation to establish options/trade-offs in financial feasibility and agricultural productivity for the farming community, against a backdrop of commercial WS-APG production. To elaborate, feasibility was measured as the difference between the total costs of harvest activities and the annual returns from the sale of agricultural produce per hectare, over a period of 3 years. A 3-year period was chosen for this hypothetical study (in line with other studies of straw incorporation impacts on soil fertility (Silgram and Chambers, 2002; Wei et al., 2015; Zhang et al., 2014) to ensure that sufficient time is provided to encourage significant changes to soil properties, yield-based performance and also to keep the uncertainty in activity costs to the minimum. The total cost of harvest is calculated by factoring-in the unit price of the energy used (red diesel), other agricultural commodities (e.g. additional fertiliser, pesticides and soil conditioners), in addition to labour costs assumed. The average annual yield of wheat grain and wheat straw (which is an indicator of soil fertility at a given fertiliser input) were the agronomic measures of this feasibility assessment. Extensive studies on the effect of wheat straw on short/long term soil characteristics and performance have been undertaken earlier (Brennan et al., 2014; Karer et al., 2013; Sadeghi and Jafar Bahrani, 2009; Shindo and Nishio, 2011).· However, the outcomes of the analysis were highly restricted to the soil-types, local weather patterns, as a result of which, outcomes of such studies were expected to be ambiguous for inclusion within this study. Due to very limited numbers of recent studies based in the UK, this study adopted data from regions of similar weather conditions and soil types but based in other parts of the world. In addition to this, a study by the Agricultural and Horticultural Development Board (Agriculture and Horticulture Development Board, 2016b), which provided a review of all UK-based literature, on the key effect of straw application, overall soil performance/characteristics and biomass yield was also adopted. A quantitative measure of soil performance with straw incorporation or straw/biochar incorporation was adopted from these references.

Further information on the uncertainties and assumption adopted for this study have been presented in the appendix section F. This agronomic study adopted three scenarios to represent the potential fate of the fraction of wheat straw harvest

Scenario 1: This is the baseline scenario where the harvested straw fraction amounts to 50% and the remaining biomass is incorporated back into the soil, in addition to WS-biochar obtainable from the baled and sold fraction of wheat straw. This corresponds to harvest of wheat straw leaving a 300 mm high stubble.

Scenario 2: The fraction of straw harvested per hectare is 75% while 25% is re-incorporated which corresponds to the practice of leaving 100 mm of straw stubble. The wheat straw that is harvested is assumed to be utilised for APG production and WS-biochar, a soil conditioner and carbon-sequestering by-product of the APG production process, is assumed to be incorporated into the soil in addition to unharvested straw.

Scenario 3: The fraction of straw harvested per hectare of 25% while 75% is assumed to be re-incorporated, leaving 500 mm straw stubble. Unlike earlier scenarios, WS-biochar incorporation is omitted for this scenario due to relatively high loading of nutrients via raw wheat straw.

The costs of each of the scenarios are highly variable (dependant on the location of the farm, soil types, weather conditions, cropland area) and it would be laborious to capture these variables into this hypothetical agronomic study. However, a qualitative discussion on the effect of these parameters was included for the reader's reference. The processes involved in these scenarios will influence their final cost, with the cost contributing factors within the post-harvest activities being fuel consumed (during straw harvest, chopping, soil preparation, agrochemical application) and quantified material consumption (pesticides, additional/discount of fertilisers for the follow-up crop). In addition to the above mentioned, a qualitative discussion on continuous removal of wheat straw in the absence of returning any organic matter or substitutes to the soil and the benefits/issues associated to this practice have been presented.

In order to overcome the uncertainties associated with this segment of economic analysis, assumptions were adopted from an environmental assessment (Lokesh et al., 2017) undertaken for WS-APG and PW-APG which are presented in the appendix section F.

2.5.1. Stage 1: baling/carting of wheat straw

In this method of straw management, straw combine-harvested with grain, was assumed to be packed and carted out of the fields by the agricultural contractors on the day post-harvest. The fuel consumed for straw harvest will primarily determine the cost for this activity. According to Špokas and Steponavičius (2010), combine-harvesting of straw (50% harvest) and grain was assumed to take up roughly 15–20% of fuel consumed per growth year which allocated to straw harvest was determined to amount to roughly 12 ± 2 l/ha.Previously published literature indicated that the rate of fuel consumption decreases (by 2–4 l/ha) with the increase in desired stubble height (for every100 mm) (Baggs et al., 2006; Powlson et al., 1985). In accordance to the influence of the above mentioned factors, in parallel to agricultural fuel use assumptions specific to our study, fuel consumption for 75% (stubble height-100 mm), 50% (300 mm) and 25% (500 mm) harvest has been extrapolated from earlier analyses (Powlson et al., 2008a) to be 15.9 l/ha, 11.3 l/ha and 8.5 l/ha respectively. Fuel consumption for baling of wheat straw has been has been adopted from prices quoted by National Association of Agricultural contractors (NAAC) (National Association of Agricultural Contractors, 2017, 2016, 2015).

2.5.2. Stage 2: straw chopping and re-incorporation

The activities that entail straw re-incorporation include straw chopping, straw spreading and ploughing. All these activities consume fuel and prices reflect fuel and service charges (National

Association of Agricultural Contractors, 2017, 2016, 2015). In addition of the activities listed below, re-incorporation takes into account a hypothetical rate of pesticide application which is expected to increase with straw incorporation due to the increased risk of slug infestation and fungal attack (Baggs et al., 2006; Powlson et al., 2008b). The rate of increase in grain yield, by 23–25%, was assumed in this study is based on previously undertaken studies (Bhogal et al., 2011; Nicholson et al., 2013; Špokas and Steponavičius, 2010). In straw incorporation, it was assumed that upon grain harvest, the straw being harvested, chopped, spread and ploughed into the soil. The cost of fuel consumed for the straw harvest was similar to that of straw-removal. The cost of chopping, spreading and ploughing were determined for the default scenario where 50% straw is incorporated and extrapolated for the varying straw harvest targets (25% and 75% harvest).

The costs associated with the activities (encompassing material/energy intensity and service charges) assumed for each of the harvest scenarios were weighed against each other. The total cost of these activities deducted from straw and grain sales would demonstrate the "environmentally-ethical and profitable" straw harvest scenario for the farmer. Quantities of material and energy requirement for each of the residue management activities have been presented in Table 2.

The costs associated with straw harvest and management are summarised in Table 3.

3. Results & discussion

3.1. Economic performance – processing

The costs incurred from resource consumption and labour have been calculated and are summarised in Fig. 5. The analysis pathway, involving the production of WS-APG was determined to be less expensive, in comparison to the baseline candidate, PW-APG. As anticipated, the biomass cultivation phase was determined to be the highest cost-contributor from mass-based allocation of costs between wheat straw and wheat grain. Use of agrochemicals and fuel contributed the highest cost to the overall biomass cultivation costs. In the case of PW-APG, the choice of functional unit, coupled with the relatively higher APG productivity per unit agricultural input, was determined to be a key factor for the baseline feedstock's relatively lower cultivations costs. To be specific, with WS-APG, 1.096 kg of wheat straw was required to synthesise 1 g of the WS-APG. Whereas, the quantity of primary feedstock required to prepare 1 g of WS-APG are relatively higher than that required to prepare 1 g of PW-APG (Lokesh et al., 2017).

The rationale for the consideration of biomass cultivation costs, for the default scenario, was to consider potential increment to the value of the "low-cost" but high-demand feedstock. Further elaboration on the scenario-based sensitivity assessment has been provided under the appropriate sections. The second-most expensive phase was the labour cost which was mainly due to utilisation of technically-skilled labour and the annual volatility in the regional inflation rates. In terms of technical costs, palm kernel and wheat grain based APG was observed to have relatively higher pre-processing costs due to relatively higher demands for resource inputs, lack of material recovery and re-use strategies and waste treatment requirements for some of the toxic process outputs. The second most-expensive phase for PW-APG was the "transportation" phase involving heavy logistics including transoceanic and rail freightage of primary and secondary feedstock.

Focussing on the process technology for WS-APG production, the pre-processing costs employs green techniques, including supercritical wax extraction and low-temperature microwave, which was determined to deliver a significant saving, bringing costs down to \$0.01/kg of WS-APG, compared to that of \$0.64/kg of PW-APG. The lower costs were primarily due to the capability of the process to recover and re-use its supercritical solvents and generation of very minimal and less-toxic wastes. However the costs associated with refining the chemical feedstock to WS-APG was determined to cost more than double the refining costs associated with the PW-APG pathway. The costs were determined to be higher due

Table 2
Quantities of material and energy inputs within post-harvest phase of wheat cultivation (over 3 analysis periods).

Parameters	Residue management activity	Material/energy	Units	Scenario 1 (default)	Scenario 2	Scenario 3
Straw harvest			kg/ha	3500	5250	1750
Grain yield[a]	*(after straw and biochar incorporation)*		kg/ha	9504	7744	9856
Straw processing	Straw harvest	*Fuel*	l/ha	11.3	15.9	8.5
	Straw baling	*Fuel*	l/ha	18.3	24.5	9.2
	Carting out	*Fuel*	l/ha	17.2	25.7	8.6
	Straw Chopping	*Fuel*	l/ha	3.76	2.84	6.18
	Straw spreading	*Fuel*	l/ha	4.30	2.15	6.45
	Ploughing		l/ha	67.28	50.46	117.76
Fertiliser	Application rate[b]	*N*	kg/ha	196	196	196
		P	kg/ha	45	45.00	45
		K	kg/ha	65.25	65.25	65.25
		Mg	kg/ha	45	45	45
Straw Nutrient content	Nutrient[c]	*N*	kg/ha	–	–	–
		P	kg/ha	29.4	14.7	44.1
		K	kg/ha	36.4	18.2	54.6
		Mg	kg/ha	9.1	4.55	13.65
		Fertiliser app. fuel	l/ha	19.9	19.9	19.9
Pesticides	Metaldehyde[d]		kg/ha	0.5	0.35	0.7
	Fungicides[d]		kg/ha	7.3	5.2	9.05
	Application fuel		l/ha	1.22	1	1.5
Soil management	Artificial conditioning	*Biochar*	kg/ha	2895.0	4342.1	1447.4

Note:
[a] Grain yield increase from continuous straw incorporation over 3 years has been adjusted. An change in grain yield has been adjusted by about +8%, −12% and +12% based on the amount of straw incorporated.
[b] Fertiliser application rate assumed to be constant over the 3 analysis years to capture the effect of straw/biochar incorporation.
[c] The average nutrient value of the straw that is harvested and baled is based on information from sources (Home Grown Cereals Authority (HGCA), 2009).
[d] Max level of metaldehyde and fungicide application suggested by the sources (Bhogal et al., 2011; Nicholson et al., 2013; Nicholson et al., 2013).

Table 3
Assumed unit cost of post-harvest operations in wheat cultivation.

Parameters		Activity costs ($/ha)[a]
Ploughing		83.67
Stubble Cultivation		58.30
Fertiliser application	*Compost*	17.25
	Liquid fertiliser spraying	21.74
	Slug pelleting	11.84
Combine harvesting		133.46
	Straw chopping	9.44
	Seeding[b]	11.48
Straw chopping	*(separate operation)*	59.65
Baling	120 × 60 cm	15.87
Carting out the bales		133.99

Note:
[a] Prices from (National Association of Agricultural Contractors, 2017, 2016, 2015).
[b] Price of wheat grain for the year 2013–2017 was adopted from DEFRA agricultural statistics $0.186/kg, $0.172/kg and $0.215/kg respectively. Price of wheat grain for the year 2013–2017 was adopted from figures published by British Straw and Hay Merchants Association $0.067/kg,$0.05/kg and $0.043/kg respectively (National Statistics- UK, 2017).

to the imbalance in the feedstock to product conversion ratio between the analysis and baseline scenario. To be specific, baseline (PW-APG) process can produce 104 kg of PW-APG from a hectare worth of feedstock compared to that of the 3.96 kg of WS-APG via the analysis process. However, it is expected that these costs will reduce in time with technical maturity and optimisation of the WS-APG pathway. Additionally, significant quantities of high-quality by/co-products result from the different stages of the WS-APG pathway including levoglucosan (finding application in pharmaceutical industry), organic acids, aldehydes and soil-conditioning straw biochar which can potentially reduce the overall cost of WS-APG production, if commercialised. In this study, production costs presented for WS-APG are attributed only to the APG synthesised.

3.1.1. Sensitivity study

A sensitivity study was undertaken to assess the impact of the three different *biomass cultivation* scenarios listed in the *methodology* section. The outcome of cost allocation within the three scenarios based on mass and economic significance has been presented in Fig. 6.

For the analysis case, the cost of biomass cultivation was determined to be the highest and the impact of three scenarios on the overall production costs was assessed. Mass-based allocation was chosen as the default towards final feasibility assessment to account for the most unlikely and the most-expensive option for production. In relation to the default scenario, allocation of costs according to the wheat straw and grain's economic significance reduces the overall production cost of WS-APG by an average −48%, as presented in Fig. 6. In the case of PW-APG, all the wheat cultivation costs has been incorporated onto the wheat grain (as should be) which increased the predicted market price by an average of +28% (varying between +8 and + 48%). This outcome inferred that potential techno-economic optimisation to the WS-APG production pathway can only have a positive impact on the total costs, compared to the baseline candidate, PW-APG, which is also being produced using an upgraded and optimised facility.

3.2. Economic resource efficiency

3.2.1. Output service quality

Some semi-quantitative resource efficiency metrics were utilised in this study to highlight the efficiency of value addition to a low-value feedstock (such as wheat straw) without undermining the value of the services and functionality. The outcome of this assessment has been presented in Fig. 7.

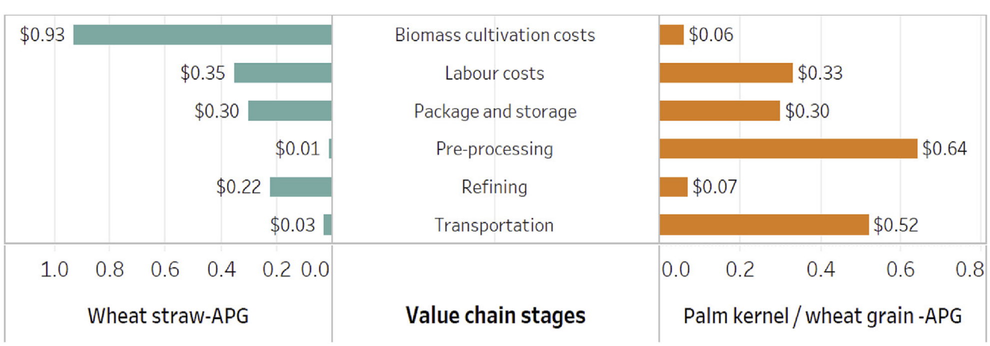

Fig. 5. Comparison of the cost of producing 1 kg of WS-APG and PW-APG from "feedstock production to factory gate".

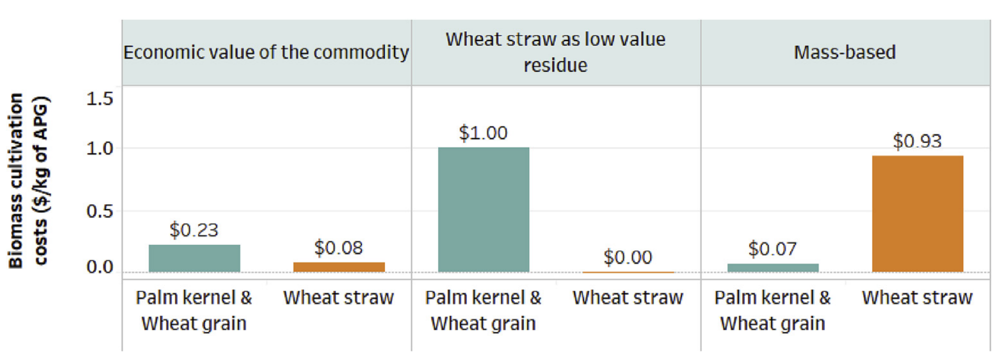

Fig. 6. Allocation of biomass cultivation costs based on the three scenarios.

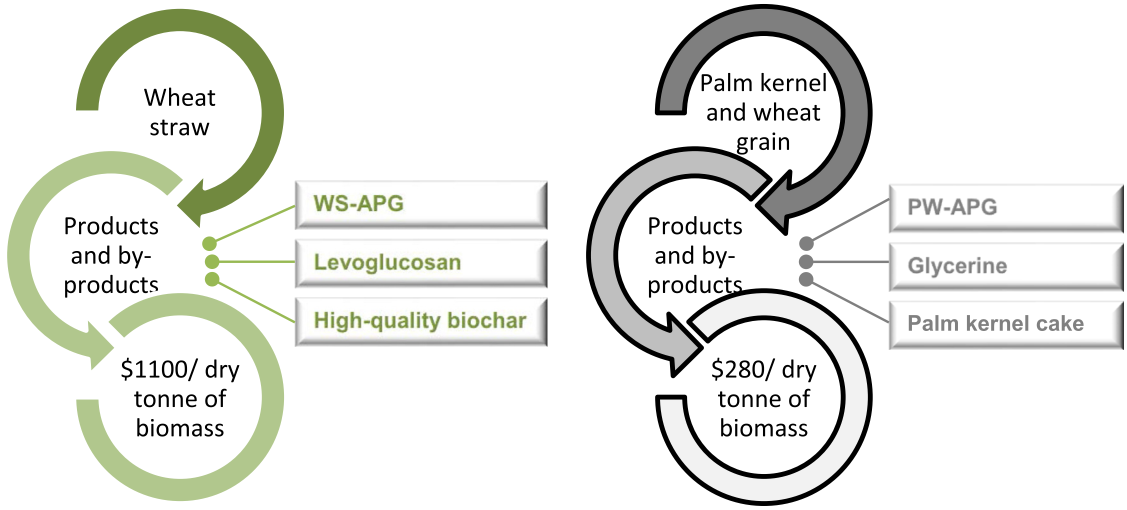

Fig. 7. Comparison of output service quality between the two APG candidates (conversion of raw-material to high value products).

The reason behind the WS-APG production method delivering relatively better economic potential stems from the current high-value application of the products and by products generated from this process. Particularly levoglucosan which finds a number of high-value application in organic chemistry and also in the synthesis of some biodegradable plastics (Budarin et al., 2009; Zhang et al., 2013). The high-quality biochar generated from low-temperature pyrolysis also finds application as a soil conditioner in horticulture and agriculture.

3.2.2. Energy efficiency

Energy efficiency is used as a measure of the amount of energy invested into creating the value-added products (primary, by-products and co-products), from an economic perspective. The energy input relative to the economic value of the products and by-products generated for both the analysis and baseline candidates has been presented in Fig. 8. In the wheat straw based process, the products and by-products generated and included within the system boundary of the process include WS-APG, Levoglucosan and Biochar. In the baseline case study, following a system boundary similar to the reference study (Guilbot et al., 2013) (Palm kernel and wheat grain), the products and by-products generated include PW-APG, glycerine (from the transesterification process) and palm kernel cake. For the purpose of clarity, the amount of energy invested into the transformation of raw material to the respective products and by-products have also been presented in Fig. 8. Roughly 935 kg per batch worth of products and by-products are generated from the “analysis” WS-process (a majority of which was biochar, followed by levoglucosan) while that generated from the “baseline PW-process amounts to roughly 800 kg per batch. When applying the energy consumption data with the total amount of products generated to equation (3), for each of the case studies, WS-based process was identified to be the most energy efficient compared to the baseline process.

3.3. Agronomic impact

A socio-economic study is undertaken, as a part of this economic impact analysis, focussing on the implications of scale up mainly encompassing feedstock supply, its long-term effects on cropland productivity and, subsequently, its long-term feasibility. The outcomes of this sensitivity study, undertaken with the consideration of the three scenarios, has been tabulated in Table 4.

From the agronomic analysis, Scenario 2, which involves 75% harvest, was determined to be the lowest cost options. However, an increase in grain yield, over a period of 3 years from continuous straw incorporation suggested scenario 1 (default) to be more sustainable and profitable in comparison to Scenario 2 or 3, in spite of a relatively increased pesticide requirement to prevent crop damage from slugs infestation. The gross revenue generated from sale of agricultural commodities (grain and straw) discounting the cost of operations for a period of 3 years with 25%, 50% and 75% straw removal was determined to be \$2199.31/ha^{-}, \$2226.41/ha, \$1993.96/ha respectively. The difference in profitability of the good agricultural practice recommended scenario 3 (25% straw removal), compared to the default scenario (50% straw removal) was superior by 0.53%. The activity which had the highest influence on total costs was ploughing the left-over straw back into the soil and this cost accounts for both fuel, equipment use and service charges. The second highest cost was contributed by a parameter N fertiliser application, which was fixed constant over the three analysis years.

This study concluded that a 50% straw harvest option was more profitable compared to that of the other two scenarios. In the short term, scenario 3 may appears to be more promising with its better returns from grain sale, however, this practice is likely to increase losses from pest and soil disease which in turn would increase the necessity to opt for synthetic pesticides, thereby leading to long-term environmental risks. Moreover, the optimal straw removal strategy from the default scenario is likely to provide for residual straw breakdown and preparation of soil for the next batch of crops. Increased level of straw removal (scenario 2), was likely to reduce yield overtime due to loss of soil organic matter, soil compaction, microbial activity to facilitate nitrogen cycling (resulting in N losses) and imbalance in physical and chemical soil characteristics.

3.4. Consideration for commercialisation

These economic feasibility analyses were undertaken for a preliminary impact evaluation of the proposed laboratory scale thermochemical process. It was observed that, from techno-economic perspective, the proposed thermo-chemical process required further optimisation for pilot and commercial level

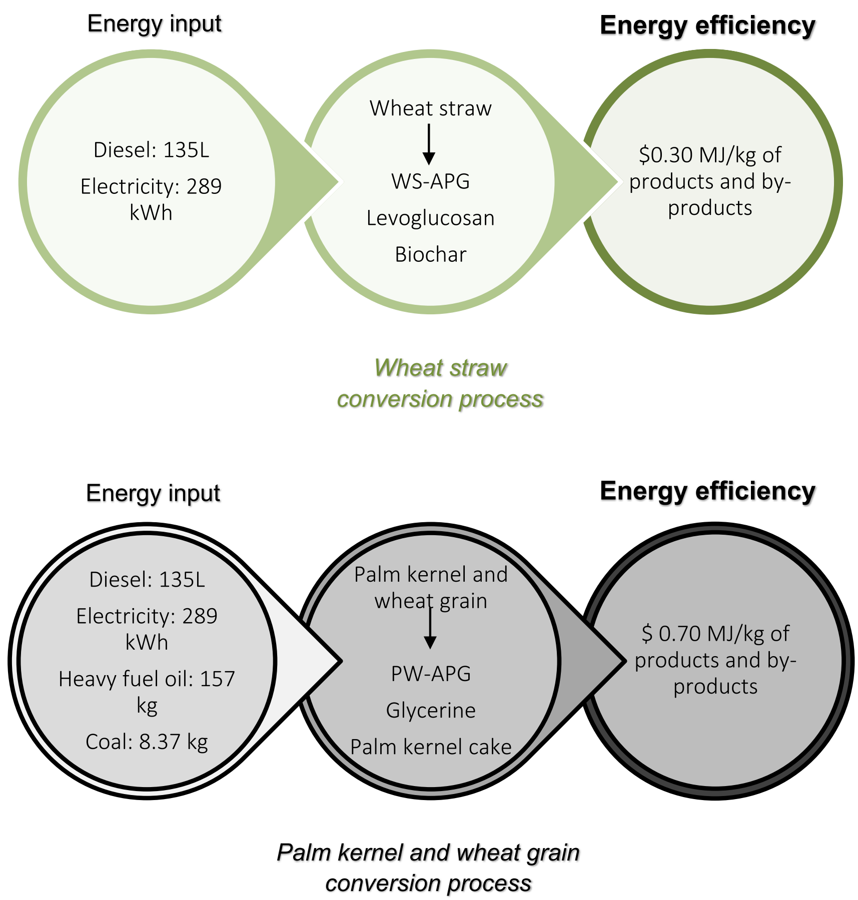

Fig. 8. Comparison of Energy efficiency attributable to the conversion of raw material to products and by-products within the WS-APG and PW-APG pathways.

Table 4
Cost of straw "bale/sale" and soil incorporation of varying levels of straw removal over a period of 3 years.

Parameters		Materials	Costs and Returns ($/ha)		
			Scenario 1 (Default: 50% removal)	Scenario 2 (75% removal)	Scenario 3 (25% removal)
Straw processing	Straw Chopping	*Fuel*	2.39	1.80	3.93
	Straw harvest	*Fuel*	7.21	10.14	5.42
	Straw baling	*Fuel*	11.68	15.60	5.76
	Carting out	*Fuel*	3.32	2.00	4.75
Fertilisers	Synthetic	*N*	64.48	64.44	64.48
		P	6.44	6.44	6.44
		K	37.36	37.36	37.36
		Mg	16.26	16.26	16.26
	Nutrient value of harvested straw *(returns)*	*N* [a]	–	–	–
		P	0.60	0.90	0.30
		K	19.02	19.02	19.02
		Mg	1.75	2.63	0.87
Pesticides	Synthetic	*Metaldehyde*	0.67	0.20	1.37
		Fungicides	1.83	1.32	2.29
Soil management	Additives	*Artificial soil conditioners* [b]	0.00	0.00	0.00
		Application fuel cost	0.77	0.64	0.96
		Ploughing cost	42.9	22.45	75.08
Total cost of operations			221.76	194.44	212.81
Sale of produce	Wheat grain sale	*@ $0.215/kg*	2051.26	1731.20	2112.72
	Wheat straw sale	*@ $0.057/kg*	175.15	262.76	87.59
Net returns			2004.57	1781.15	1994.01

Note:
[a] Nitrogen content of harvested straw unknown and hence, omitted. Standard N application rate assumed over 3 years.
[b] Artificial soil conditioners refer to incorporation of biochar (a by-product of wheat straw APG synthesis). Biochar is assumed to be delivered to the farmers free of cost as compensation for the wheat straw that is removed, baled and sold for WS-APG production.

production. Techno-economic improvisation to the analysis (WS-APG) pathway could lower the overall costs by encouraging a more efficient and optimised production strategies. Production costs could be reduced further through via the following strategies.

- Sourcing "used" wheat straw from animal husbandry which is likely to reduce feedstock costs on the overall production costs: a biomass-cascading opportunity;
- Optimisation of technical performances within the stages, which includes use of relatively less-expensive and low impact green solvents, improving process efficiencies by boosting the specificity of the process and lowering by-product waste generation by adopting suitable low-impact catalysts;
- Economic optimisation of biomass (wheat straw-a relatively less-dense feedstock) transportation costs scaling up (savings from bulk material/service purchases) through establishment of a local small/medium level infrastructure.

We acknowledge that the impacts of straw/biochar incorporation depend on a variety of uncontainable factors, especially local weather patterns and soil conditions. Therefore, there were no representative data to quantify the residue incorporation impacts on soil health/returns and any variations in these assumptions will have a significant impact on the outcome, regarding the agricultural productivity, presented in this study. A prospective socio-economic evaluation focussing on the impact of the high quality derivative of the WS-APG process, straw biochar, on different UK soil types and quantifying the rate of soil health improvement over long term would be able to address the uncertainty embedded in the outcome of the agronomic analysis. In fact, this level of assessment undertaken for any bio-based value chain will shed some light on the socio-economic compatibility of the value chain with the interest of the local activities/farming community. For now, this paper concludes that process commercialisation could reduce the production costs and the outcome of this quantitative economic impact assessment inferred that the thermo-chemical pathway devised for the production of wheat straw-APG was a promising alternative to conventional bale and sale of wheat straw for other purposes.

3.4.1. Limitations

Though this paper has arrived at the suggested outcome, the main deliverable of this paper is a methodology for the economic feasibility evaluation of early-stage promising bio-based product that have been developed for potential commercialisation. It is essential to note that the outcome of the assessment presented under appropriate section (economic feasibility, resource efficiency and agronomic impacts) are applicable only to the assumptions adopted within the boundary of the study. As applicable to any economic feasibility assessment, variations to some of the assumptions based on uncontrollable parameters, (for example, sudden shocks in the market dynamics and its impact on commodity prices, labour rates and any trade related instabilities, and also in terms of the agronomic evaluation, the impact of climate change on soil quality, weather patterns, rate of straw biodegradation and associated boost in yield), could impact to the outcomes presented in the paper.

4. Conclusion

An economic feasibility evaluation of a green pathway, devised to synthesize high value chemical (alkyl polyglucoside) from renewable and low cost wheat straw, was undertaken from a life cycle ('farm-gate') perspective. An existing commercial pathway of APG production from palm kernel/wheat grain was chosen as a benchmark, owing to the innovative nature of the analysis process. The suggested green approaches to produce APG from wheat straw (WS-APG) was determined to be the cheaper option, in comparison to that of the baseline case study (PW-APG). Some novel resource efficiency methodologies, conventionally utilised for the selection of bioenergy candidates but adapted for bio-products synthesised in this study have been proposed. They were measured as output service quality and energy efficiency where the analysis process was determined to be 77% more rewarding and 72% more energy efficient compared to the baseline palm kernel and wheat grain based process, in accordance to the assumptions adopted for this study. A socio-economic assessment was also undertaken to assess the benefits of potential process scale-up of wheat straw-APG production and its impact on the ecological/economical trade-offs that would potentially be considered by the practicing farming community. This segment has an agronomic basis where the potential ecological and economic impacts of 25% 50% (baseline) and 75% wheat straw harvest was assessed, adopting specific assumptions to handle uncertain parameters such as effects of local weather pattern and soil type. This semi-quantitative agronomic analysis infers that 50% wheat straw harvest was more profitable relative to 25% or 75% straw harvest due to its optimal ecological (soil organic matter, microbial activity and productivity) and subsequent economic (revenue from grain and straw) contributions to the agricultural community.

Declaration of interest

None

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Abbreviation

GHG	Greenhouse Gas
UN SDGs	United Nationals Sustainability Development Goals
AHDB	Agricultural and Horticultural Development
APG	Alkyl polyglucoside
CH4	Methane
CO2	Carbon-dioxide
ECHA	European Chemical Agency
EEA	European Environmental Agency
H2O	water vapor
HGCA	Horticultural Grown Cereals Authority
kT	kilotonnes
LCA	Life cycle assessment
LCC	Life cycle costing
NAAC	National Association of Agricultural contractors
NaOH	Sodium hydroxide
PW-APG	Palm kernel and Wheat grain APG
REACH	Registration, Evaluation, Authorization, restriction of Chemicals
ScCO2	Supercritical carbon-dioxide
WS-APG	Wheat straw derived APG
PW-APG	Palm Kernel and Wheat Grain based APG

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2018.10.220.

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