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5 **Process integration, energy and GHG emission analyses of Jatropha-based biorefinery**
6 **systems**

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12 **ABSTRACT**

13 Driven by the need to develop a wide variety of products with low environmental impact,
14 biorefineries need to emerge as highly integrated facilities. This becomes effective when overall
15 mass and energy integration through a centralised utility system design is undertaken. An approach
16 combining process integration, energy and greenhouse gas (GHG) emission analyses is shown in
17 this paper for Jatropha biorefinery design, primarily producing biodiesel using oil-based
18 heterogeneously catalysed transesterification or green diesel using hydrotreatment. These processes
19 are coupled with gasification of husk to produce syngas. Syngas is converted into end products,
20 heat, power and methanol in the biodiesel case or hydrogen in the green diesel case. Anaerobic
21 digestion of Jatropha by-products such as fruit shell, cake and/or glycerol has been considered to
22 produce biogas for power generation. Combustion of fruit shell and cake is considered to provide
23 heat. Heat recovery within biodiesel or green diesel production and the design of the utility (heat
24 and power) system are also shown. The biorefinery systems wherein cake supplies heat for oil
25 extraction and seed drying while fruit shells and glycerol provide power generation via anaerobic
26 digestion into biogas, achieve energy efficiency of 53% in the biodiesel system and 57% in the

green diesel system. These values are based on high heating values (HHV) of *Jatropha* feedstocks, HHV of the corresponding products and excess power generated. Results showed that both systems exhibit an energy yield per unit of land of 83 GJ ha⁻¹. The global warming potential from GHG emissions of the net energy produced (i.e. after covering energy requirements by the biorefinery systems) was 29 g CO₂-eq MJ⁻¹, before accounting credits from displacement of fossil-based energy by bioenergy exported from the biorefineries. Using a systematic integration approach for utilisation of whole *Jatropha* fruit, it is shown that global warming potential and fossil primary energy use can be reduced significantly if the integrated process schemes combined with optimised cultivation and process parameters are adopted in *Jatropha*-based biorefineries.

Keywords: biodiesel, green diesel, biorefinery, utility system design, LCA, process integration.

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1. Introduction

Jatropha curcas as feedstock for the production of biofuels has been explored in recent years in tropical countries (such as India, China, Malaysia, Indonesia, Mozambique, Brazil, Mexico, etc.) with about 12 000 km² of plantations globally in 2011 [1]. In order to establish *Jatropha curcas* as a competitive energy crop, the whole fruit must be exploited by extraction of valuable components and conversion into added value products [2],[3]. This can be achieved in integrated biorefineries as shown for other feedstocks such as wheat [4]. Major *Jatropha* fruit fractions include fruit shells, seed husks, oil and cake after oil extraction from the kernel, presented along with compositions and energy values in **Table 1**. *Jatropha* oil has been extensively investigated for biodiesel production (with glycerol co-production) using homogeneous and heterogeneous catalysis [5], [6]. Heterogeneous catalysts (e.g. MgO, CaO, zeolites) facilitate separation of products and provide greater flexibility to free fatty acid content in oil [6]. An alternative to biodiesel is green diesel, which is produced by hydrotreatment of vegetable oils. Propane fuel is also generated as co-product from this process [7]. This process has the advantage of the biofuel products being readily

adaptable to current infrastructure. Throughout the paper, the term biodiesel is used to indicate the diesel produced by transesterification. Green diesel is the diesel produced by hydrotreatment.

Table 1

Conversion of the whole *Jatropha* fruit (not only the oil) into energy products (biofuel, heat, power) has more energy output than only biofuel production from the oil [8]. The suitability of extraction cake as an added value product has been studied [9]–[14]. It has been shown that cake from toxic *Jatropha* genotypes needs detoxification prior to its use as a valuable source of protein and potential substitute for soy meal in animal feed [11], [13]. However, non-toxic genotypes as those native to Mexico make the extraction cake suitable for animal feed [9], [10]. An alternative use of *Jatropha* cake is as an organic fertiliser [12], [14], [15]. Cake and fruit shells are a good substrate for anaerobic digestion into biogas [16]–[18]. The glycerol generated as co-product in the biodiesel production process has also been studied as a potential feedstock for biogas generation [19], [20]. *Jatropha* seed husk has been explored as an attractive feedstock for gasification and pyrolysis [8], [21], [22]. These thermochemical processes can produce syngas for the generation of liquid fuels, chemicals, heat and power from residues [23]–[29]. This opens process integration opportunities in the biorefinery to produce required raw materials such as methanol (used in the transesterification of *Jatropha* oil to produce biodiesel) or hydrogen (used in the hydrotreatment of vegetable oil to produce green diesel) internally. With systematic selection and process integration of co-production routes, fossil energy use and global warming impact of biorefineries can be reduced [25]–[29]. Life cycle assessment (LCA) is an effective tool for analysing material and energy inventories and environmental impacts throughout a product or process life cycle [30]–[35]. LCA studies of *Jatropha*-based bioenergy systems showed that reductions in greenhouse gas (GHG) emissions in the range of 55%–90% with savings in cumulative fossil primary energy (CPE) of more than 70%, in respect to a reference fossil-based system are achievable by converting the various *Jatropha* fruit fractions [5], [32]–[35]. Although these studies considered utilisation of various *Jatropha* fruit

fractions and various conversion routes, potential benefits from process integration opportunities have not been explored. Starting with an effort to improve energy efficiency of process industries in 1970s, the process integration tools [36]–[41] have been widely applied with valuable contributions in the field of biorefineries such as process synthesis [39], [40], heat and mass integration [23]–[25], pollution and GHG emission control [41], optimisation of process and supply chain [42], and of energy and material efficiency for reduced energy consumption [43]. This work proposes an effective framework combining process integration tools and LCA approach for more resource efficient biorefinery design. It is a matter of urgency to investigate systematic process integration synergies and compare the energy and global warming impact from greenhouse gas (GHG) emissions between biorefinery integration alternatives. This paper shows comparison of GHG emissions and energetic efficiencies between green diesel and biodiesel productions from integrated Jatropha biorefinery systems in which the required electrical and thermal energy and hydrogen or methanol are generated from Jatropha residues.

2. Methodology

2.1 Goal and system definition

The objective of this work is to produce integrated biorefinery schemes from Jatropha fruit for the production of biofuels, power and co-products and assess their GHG emissions and cumulative primary energy (CPE) using life cycle analysis. The energy efficiency is also assessed. The assessment is to show the need and advantages that can be obtained from optimisation of system parameters (such as yields and energy efficiencies), process integration and the use of advanced technologies for future deployment.

Fig. 1 presents an overview of the systems considered in this study. Two alternative biofuel production systems are studied: biodiesel and green diesel. The base case comprises the standalone biofuel plants wherein the oil is the only Jatropha fruit fraction, converted into either biodiesel and glycerol or green diesel and a propane fuel mix (a mixture mainly composed of propane and some

CO₂), with the oil extraction cake as a by-product in both cases. In these stand-alone systems, any utility requirements, after internal process integration, are supplied from fossil sources.

In the ‘integrated biodiesel or green diesel systems’, the husk is gasified into syngas which is used to supply heat and power, along with either methanol for biodiesel or hydrogen for green diesel productions. Any excess heat is converted into power via steam generation. The excess power is then exported to the electricity grid. In the base case and the integrated systems, the glycerol and propane are exported as fuels and the cake as animal feed. As shown in **Fig. 1**, five alternatives for the use of fruit shells, extraction cake and glycerol within the integrated systems are proposed for the whole *Jatropha* utilisation to improve conversion efficiency:

1) Cake is burned to supply heat for oil extraction (wherein natural gas is substituted) and seed drying (wherein diesel is substituted).

2) Fruit shells are used as fuel to provide heat for oil extraction and seed drying. Cake is used as fertiliser replacing part of the inorganic fertilisers currently used.

3) The same as alternative 2, but cake is sold as animal feed. Soy meal is replaced by the cake.

4) Cake, fruit shells and glycerol in the biodiesel case, are used in anaerobic digestion. The biogas produced is converted into electricity.

5) Cake supplying heat for oil extraction and seed drying as in alternative 1. The fruit shells and glycerol in the biodiesel system are used as in alternative 4.

Fig. 1 Overview of the integrated *Jatropha* biorefinery systems for the production of biodiesel and green diesel with utilities and auxiliary raw materials generated from *Jatropha* by-products. Numbers 1–5 indicate in which alternative the options for by-product utilisation are selected. Mass flow rate in Gg y⁻¹, heat and electricity in PJ y⁻¹. IBGCC: Integrated biomass gasification and combined cycle

Substitution approach by taking credits from co-products has been used. GHG emissions have been characterised by their global warming potential (GWP) impact as CO₂-eq. The biorefinery is assumed to be located within the radius of plantations of the non-toxic genotype in Michoacan, Mexico. Transportation distance for fruit shells, seeds and cake is equal to the radius of the plantation land assuming a circular shape. The transportation of auxiliary raw materials and

biorefinery products are assumed to be 100 km. The cumulative primary energy (CPE) and GWP factors are based on road transportation using 100% fossil-based diesel [45]. The embodied CPE and GWP impact of the various fuels and raw materials are extracted from various sources [45]–[49] and are presented in **Table 2**. The fossil-based cumulative primary energy and environmental impact data for power are deduced from [46] and the Mexican national electricity mix data (natural gas = 51.8%, fuel oil = 16.7%, coal = 12.4%, diesel = 0.5%, renewable = 14.1% and nuclear = 4.5% by energy) [50].

Table 2

2.2 Modelling approaches for inventories

The systematic analysis comprises detailed modelling for the *Jatropha* cultivation, including seed yield modelling, and seed drying and conditioning using spreadsheet calculations. Spreadsheet based models were also used for seed processing, anaerobic digestion and biogas conversion to power. Process simulations using Aspen Plus[®] were developed to estimate the inventories from the various conversion processes. The basis for the mass and energy balances is the production of 100 Gg y⁻¹ of biodiesel from 104.7 Gg y⁻¹ of *Jatropha* oil. The same amount of *Jatropha* oil produces 93.4 Gg y⁻¹ of green diesel. These amounts also set the mass and energy flow rates of all other *Jatropha* fractions and by-products based on the yields provided in **Table 1**. Final results are then shown for 1 MJ of biofuel production for comparison. However, results are also shown in other transferrable units such as per unit of land or per unit of mass for comparisons with equivalent systems. The results from *Jatropha* cultivation and seed processing are common to all the alternatives studied (standalone and integrated systems). Raw material and energy inventory data are then extracted for overall system GWP and CPE assessments. The various modelling approaches required by the main subsystems in the overall *Jatropha* system are presented as follows.

2.2.1 *Jatropha* yield model and cultivation system

157 An empirical model correlating seed yield to average annual rainfall (AAR) and nitrogen
 158 fertilisation rate is shown using reported seed yield from field experiences around the world
 159 presented in **Table 3**.

160 **Table 3**

161 The annual seed yields at maturity Y_{mat} in kg ha^{-1} ; 1 ha= 0.01 km^2) under natural conditions, i.e.
 162 without nutrient or water management, in **Table 3** were determined from the Chapman–Richards
 163 correlation shown in **Eq. 1** [51]. Y_{age} in (kg ha^{-1}) is the yield at a given plant age (A) and the model
 164 coefficients for Jatropha are $b=0.852$ and $c=3.466$ [51].

$$Y_{age} = Y_{mat} (1 - e^{-bA})^c \quad (1)$$

165
 166 Assuming that the yield values in **Table 3** are for Jatropha grown under rain fed conditions, the
 167 calculated values of Y_{mat} are correlated to AAR. A third order polynomial function can applied to fit
 168 the data in **Table 3** as shown in **Eq. 2**

$$Y_{mat}^{AAR} = a_1 AAR^3 + a_2 AAR^2 - a_3 AAR \quad (2)$$

170 Y_{mat}^{AAR} is the annual seed yield at maturity (in kg ha^{-1}) and a given AAR (in mm). The values of the
 171 polynomial constants are $a_1 = -5.6163 \times 10^{-6}$, $a_2 = 1.3663 \times 10^{-2}$ and $a_3 = 5.2481$.

172 The annual seed yield at maturity considering nitrogen fertilisation is correlated to its base value at
 173 annual average rainfall of a location and the nitrogen fertilisation rate. The resulting function is
 174 shown in **Eq. 3**. This equation was developed based on conditions [53], similar to plantations
 175 located in Michoacan, Mexico.

$$Y_{mat}^N = Y_{mat}^{AAR} + b_1 (1 - e^{-b_2 N}) - b_3 N \quad (3)$$

177 Y_{mat}^N (in kg ha^{-1}) is the annual seed yield at maturity considering nitrogen fertilisation. N is the
 178 nitrogen fertilisation rate (kg ha^{-1}). The values of the constants are $b_1=2142$, $b_2=0.046$ and
 179 $b_3=1.096$.

180 The Jatropha field measurement from a plantation in Michoacan, Mexico was used as a test case to
 181 validate the model. A nitrogen fertilisation rate of 162 kg ha^{-1} is applied and the AAR of the location

182 is 900 mm. Doing a backward calculation from **Eq. 3** to **Eq. 1**, the estimated seed yield in the fifth
183 year was $Y_{age} = 4010 \text{ kg ha}^{-1}$. The observed annual seed yield is $Y_{age} = 4000 \text{ kg ha}^{-1}$ in the fifth year.
184 Comparing the predicted and observed value of Y_{age} , the error was 0.25%.

185 The plantation in Michoacan, Mexico used for model validation above was taken as a basis for CPE
186 and GWP assessment of Jatropha cultivation. The different stages in a Jatropha cultivation system
187 are shown in **Fig. 2**. A lifespan of 24 years was considered including four years to allow plants to
188 reach maturity (establishment stage). The inventories in the Jatropha cultivation are summarised in
189 **Table 4**. The estimated seed yield at maturity of 4213 kg ha^{-1} , from the yield model, was employed
190 in LCA calculations. This value is well within the range of reported maximum yields. The
191 theoretical maximum for managed cultivations under optimum conditions has been estimated as
192 7800 kg ha^{-1} [15]. The maximum yields of 4500 kg ha^{-1} in Nicaragua [54] and about 9000 kg ha^{-1}
193 in Thailand [55] were reported for managed cultivations.

194 **Fig. 2** The Jatropha cultivation system producing seeds conditioned in field

195 **Table 4**

196 The energy yield produced in the form of seeds is 114.3 GJ ha^{-1} and in the form of fruit shells is
197 32.7 GJ ha^{-1} , respectively (based on the heating values given in **Table 1**). The land use requirement
198 for the production of 104.7 Gg y^{-1} of oil is about 64385 ha (644 km^2). The calculated radius is 14.3
199 km for the Jatropha seed production of 271.2 Gg y^{-1} required for the extraction of 104.7 Gg y^{-1} of
200 oil. This is the transportation distance assumed for seeds, shells and cake. Actual distances
201 considering the non-linearity of the transportation roads can be used if known. Alternatively a
202 sensitivity analysis is recommended. However, the contribution from transportation to the total CPE
203 and GWP of the biofuel systems were found to be less than 1% (see **Fig. 9**).

204 **2.2.2 Seed processing**

205 Dried seeds transported to the biorefinery plant are first dehusked into kernel and husks. Kernels are
206 sent to an integrated solvent oil extraction process producing high quality oil and dried cake. In the
207 stand alone systems, the seed husks are not considered as a co-product. Inventories consist of

electricity, heat and make-up hexane and were determined according to [56]. The values in the reference were transformed from a seed mass basis to a kernel mass basis.

2.2.3 Biodiesel plant

Inventories of a biodiesel plant were determined by simulating the plant in Aspen Plus in **Fig. 3**, based on process specifications in **Table 5**. Oil was modelled as a mixture of tryglycerides (TG) made up of four major fatty acid components (triolein, tripalmitin, trilinolein and tristearin) and free fatty acids (FFA) content as oleic acid. Oil composition is shown along with the mass balance in Table 9 in the Appendix. Component properties were predicted using the UNIFAC-Dortmund model [57].

Fig. 3 Simulation of biodiesel production plant by heterogeneous transesterification of Jatropha oil
Table 5

A transesterification process was considered using calcium oxide as a solid heterogeneous catalyst at 70°C and a methanol-to-oil molar ratio of 9. The conversion of triglycerides is 93% and of the free fatty acids is assumed to be 100% [6]. Excess methanol was recovered by vacuum distillation and recycled. Distillation facilitated downstream separation between glycerol and methyl ester phases in a decanter. Thus, water washing and neutralisation reactors required in a typical homogeneously-catalysed process were avoided. It is assumed here that glycerol is sold as fuel. Heat integration was carried out using hot and cold composite curve analyses [36]. The reaction mix stream was preheated by the bottom stream of the methanol recovery column, before entering the transesterification reactor. The crude biodiesel stream fed to the recovery column was preheated by the distillate biodiesel stream. After heat recovery, 0.11 PJ y⁻¹ of medium pressure (MP) steam and 0.04 PJ y⁻¹ of high pressure (HP) steam were required.

2.2.4 Green diesel plant

Jatropha oil conversion to renewable or green diesel was simulated based on NREL (US) studies, which were validated against pilot plant results [7]. **Fig. 4** shows the flowsheet for the green diesel process. The same amount of oil feed (104.7 Gg y⁻¹) as in the biodiesel plant was inputted to the

simulation. The mass balance is shown in Table 10 in the Appendix. Hydrogen from natural gas steam reforming was supplied to the plant. The yield fractions and the complete set of specifications for the simulation are summarised in **Table 6**. Green diesel was modelled as $C_{18}H_{38}$. 0.027 kg of fresh H_2 and 0.028 kg of LP steam (0.5 MPa) were required for the processing of 1 kg of Jatropha oil. 93.4 Gg y^{-1} of green diesel was separated through flashing and stripping with low pressure (LP) steam. Thus, 1.121 kg of Jatropha oil is required to produce 1 kg of green diesel. 3.4 Gg y^{-1} of propane fuel is co-produced. The process incurred a direct CO_2 emission per unit of mass of green diesel equal to 0.12 kg kg^{-1} .

Fig. 4 Simulation of green diesel production plant by hydrotreatment of Jatropha oil

Table 6

2.2.5 Husk gasification systems

The proposed integrated biomass gasification and combined cycle (IBGCC) scheme converts seed husk in an allothermal gasifier into a gas rich in hydrogen and CO [24]. The gasifier comprises of a fluidised bed steam gasification reactor and a char combustor for indirect heating of the steam gasification reactor. After gas clean-up, the syngas was converted into heat, power and methanol or hydrogen production. Integrated gasification systems for production of energy and chemicals have been found economically feasible under the proper conditions of feedstock and product prices and economic and environmental policies [23]–[25]. Jatropha seed husk, with an elemental analysis in **Table 1** and a proximate analysis (in mass fraction) made up of moisture (10.75%), volatile matter (63.40%), fixed carbon (22.30%) and ash (3.54%), formed a basis for the estimation of the primary pyrolysis product yields as in [24]. The simulation was carried out for 91.4 Gg y^{-1} of seed husk resulting from the seeds processed into oil. The simulation flowsheets of the husk IBGCC plants for methanol (IBGCC-MeOH) or hydrogen (IBGCC- H_2) production are shown in **Fig. 5** and **Fig. 6**, respectively. Mass balances are shown in the Appendix. The equipment specifications are shown in **Table 7**. A water gas shift reactor (WGSR) was coupled to the gasifier to adjust the required syngas composition for methanol or hydrogen co-production. From a sensitivity study, a steam to biomass

260 mass ratio of 0.34 was required in the case of methanol co-production and of 0.7 in the case of
261 hydrogen co-production. No additional steam was required for the WGSR.

262 **Fig. 5** Simulation of Jatropha seed husk IBGCC-MeOH plant

263 **Fig. 6** Simulation of Jatropha seed husk IBGCC-H₂ plant

264 The gas after removal of H₂S and CO₂ was further conditioned to a stoichiometric number suitable
265 for methanol [23] as well as hydrogen-rich syngas production. The clean syngas was purified in a
266 pressure swing adsorption (PSA) unit for hydrogen production. The remaining syngas (i.e. after
267 meeting the demands for methanol or hydrogen as well as the off-gas streams from methanol and
268 hydrogen separation processes) were sent as fuels to the combustor. The off-gas from PSA was
269 compressed before feeding to the combustor (**Fig. 6**). A part of the combustion heat was used in the
270 gasifier and the rest was recovered into heat and power generation via steam.

271 **Table 7**

272 The methodology for heat integration and heat and power network design is shown in [23], [24].
273 The design procedure encompasses the pinch analysis for process to process heat recovery network
274 design. Any excess heat is extracted into steam generation. The superheated steam generation must
275 be maximised at the highest pressure level, such as very high pressure (VHP) steam. Thereafter,
276 lower pressure superheated steam can be generated if heat is available at lower pressure level. To
277 ensure feasible heat integration, minimum temperature difference between hot and cold streams
278 must be maintained. The resulting heat and power design is shown in section 4.

279 **2.2.6 Anaerobic digestion and biogas power**

280 Anaerobic digestion of Jatropha by-products and residues were modelled based on reported biogas
281 yields from literature in spreadsheets. The biogas production (with CH₄ volume fraction of 70%) of
282 0.546 Nm³ from 1 kg of fruit shell [17] and 0.347 Nm³ from 1 kg of dry cake [16] was taken as the
283 basis. In the biodiesel system, 1 kg of glycerol was also digested into 0.306 m³ of CH₄ (volume
284 fraction of methane in the biogas is 68.8%) [19]. Note that these values are obtainable by optimising
285 the process (e.g. 69.4 % methane has been obtained from the cake by using an iron additive [58]). A

286 2% biogas loss due to leakage from digester was assumed and the GWP from the methane (25 g
 287 CO₂-eq g⁻¹ CH₄) has been taken into account. Biogas is used as fuel to generate electricity in a
 288 combined cycle with an efficiency of 50%. Alternative 4 is used to show the previous
 289 considerations. The alternative 4 in the biodiesel system involves anaerobic digestion of Jatropha
 290 cake, fruit shells and glycerol and power production from the resulting biogas. About 98 Gg y⁻¹ of
 291 biogas can be produced by digesting the three substrates. About 2 Gg y⁻¹ (1.97×10⁶ Nm³ y⁻¹) of
 292 biogas is lost. The GHG emissions in this biogas leakage are not completely balanced by the CO₂
 293 captured by the Jatropha plants because methane has a GWP of 25 g CO₂-eq g⁻¹. The total GWP
 294 from methane is 22.3 Gg y⁻¹. However, the methane carbon (0.68 Gg carbon y⁻¹) is captured as CO₂
 295 by the Jatropha plants and corresponds to 2.5 Gg CO₂ y⁻¹. Thus, there is a net GWP of 19.8 Gg
 296 CO₂-eq y⁻¹ from the anaerobic digestion due to biogas leakage. The remaining 96 Gg y⁻¹ (9.66×10⁷
 297 Nm³ y⁻¹) of biogas contains about 2.43 PJ y⁻¹ and is converted into 1.21 PJ y⁻¹ of electricity
 298 generation. The waste heat from the biogas power plant is used to meet heating requirements of the
 299 digester and part of the electricity is used for pumping and stirring. The heat and power
 300 requirements are according to [20], assuming a 12% of substrate content in the slurry fed to the
 301 digester. The net exported electricity was 1.10 PJ y⁻¹. In the integrated green diesel biorefinery
 302 system with alternative 4, the cake and shells were anaerobically digested. The GWP from
 303 anaerobic digestion was 18.9 Gg CO₂-eq y⁻¹. The resulting net exported electricity was 1.04 PJ y⁻¹.

304 **3. Results and discussion – Jatropha cultivation and standalone systems**

305 **3.1 Jatropha cultivation**

306 **Fig. 7** shows the resulting CPE and GWP impacts from Jatropha cultivation. The main contribution
 307 to the CPE impacts is from the manufacture of fertilisers, seed conditioning and storage. The GWP
 308 impact is mainly contributed by the field emissions due to nitrogen fertilisation, manufacture of
 309 fertilisers and seed conditioning. The cultivation system requires 0.14 PJ y⁻¹ of diesel, 0.25 PJ y⁻¹ of
 310 heat and 1970 GJ y⁻¹ of power. The CPE and GWP impact allocations to seeds are 5.4 MJ_CPE kg⁻¹
 311 ¹ and 0.63 kg CO₂-eq kg⁻¹, respectively. The CPE from Jatropha cultivation is 0.37 MJ_CPE MJ⁻¹

312 and the GWP is 43.2 g CO₂-eq MJ⁻¹ in the case of biodiesel energy. The CPE from Jatropha
313 cultivation is 0.34 MJ_CPE MJ⁻¹ and the GWP is 40.0 g CO₂-eq MJ⁻¹ in the case of green diesel
314 energy.

315 **Fig. 7** Results of a) CPE and b) GWP impacts from Jatropha cultivation

316 3.2 Stand-alone biodiesel and green diesel plants (base cases)

317 The co-products from stand-alone biodiesel and green diesel plants are the extracted cake, glycerol
318 (in biodiesel plant) and propane fuel mix (PFM, in green diesel plant). The fossil-based equivalent
319 products are fuel oil for glycerol and liquefied petroleum gas (LPG) for PFM. In the case of cake
320 being used for animal feed, 1 kg of cake could replace 1.4 kg of soy meal according to protein
321 content comparisons [11]. The inventory and impact analyses for the various processes are
322 discussed as follows.

323 0.40 PJ y⁻¹ of heat and 0.06 PJ y⁻¹ of power were required for seed processing. The CPE from seed
324 processing (a total of 0.78 PJ_CPE y⁻¹) was contributed by hexane by 5.2%, natural gas for heat
325 production (at 70% efficiency) by 75.1% and power by 19.7%. The GWP (a total of 46.7 Gg CO₂-
326 eq y⁻¹) contributions from these sources were 2%, 75.8% and 22.1% respectively.

327 The cradle-to-gate LCA results for the biodiesel standalone production system are presented in
328 **Table 8**. The GWP impact from biodiesel production was 43.3 g CO₂-eq MJ⁻¹, leading to 42%
329 saving in respect to diesel. The CPE per unit of energy in biodiesel was 0.51 MJ_CPE MJ⁻¹, leading
330 to 54% saving in respect to diesel. The operating energy efficiency, E_{op} = Energy output in all
331 products / (Energy content in all feedstock + direct energy consumption) is 91%.

332 **Table 8**

333 The LCA results for the cradle-to-gate green diesel standalone production system are presented in
334 **Table 8**. A GWP of 39.9 g CO₂-eq MJ⁻¹ was estimated for green diesel. This result is comparable to
335 the value of 45.5 g CO₂-eq MJ⁻¹ for green diesel from soybean oil reported in [7]. The resulting
336 GWP saving was 46%. The CPE per unit of energy in green diesel was 0.56 MJ_CPE MJ⁻¹,
337 resulting in a saving of 52% with respect to diesel. About 85% of the CPE and GWP impacts

338 resulted from the imported hydrogen (hydrogen is assumed to be produced from natural gas [48]).
 339 Contribution from power generation to CPE and GWP impacts is 10.7% and 11.1%, respectively.
 340 The contribution from MP steam production is 3.2% to CPE and 2.9% to GWP. The rest is
 341 contributed by LP steam production. Energy input is 0.02 PJ y⁻¹ as heat, 0.03 PJ y⁻¹ as power, 0.40
 342 PJ y⁻¹ as hydrogen (High Heating Value (HHV)=141.8 MJ kg⁻¹) and 4.15 PJ y⁻¹ as oil (HHV=39.63
 343 MJ kg⁻¹). The energy contained in green diesel (HHV=45.80 MJ kg⁻¹) is 4.28 PJ y⁻¹ and in PFM
 344 (HHV= 46.26 MJ kg⁻¹) is 0.16 PJ y⁻¹. Thus, the operating energy efficiency of Jatropha utilisation
 345 in the process is $E_{op} = 96\%$.
 346 However, the overall system includes the energy required in cultivation (0.39 PJ y⁻¹ in Section 4.1),
 347 seed processing (0.47 PJ y⁻¹ in Section 4.2.1) as well as the energy wasted in seed husk (1.82 PJ y⁻¹)
 348 ¹), fruit shells (2.11 PJ y⁻¹) and extraction cake (1.37 PJ y⁻¹). By considering all this energy inputs,
 349 the energy efficiency of the green diesel standalone plant is just $E_{op} = 4.44/10.76 = 41\%$. Similar
 350 calculations show that the energy efficiency of the biodiesel standalone plant is 39%. These results
 351 indicate a potential for improving the efficiency of Jatropha conversion for energy production in
 352 both biofuel production systems.

353 4. Results and discussion – integrated biorefinery systems

354 4.1 Process integration for GWP and CPE reduction

355 The heat and power networks of the proposed schemes for Jatropha-based integrated biorefineries
 356 were designed to meet the heat and methanol or hydrogen demands of the respective biofuel plants.
 357 Any excess heat energy recovered via steam generation is converted into power generation
 358 displacing the grid electricity. The resulting heat and power generation flowsheets are shown in **Fig.**
 359 **8** and described as follows:

360 **Fig. 8** Heat and power network of husk processing into a) IBGCC-MeOH and b) IBGCC-H₂

- 361 • The steam levels were set by the temperature levels of the various processes. Very high
 362 pressure (VHP) steam at 10 MPa and 650 °C, medium pressure (MP) steam at 1.5 MPa and low
 363 pressure (LP) steam at 0.5 MPa were generated in both IBGCC-H₂ and IBGCC-MeOH systems.

364 • High pressure (HP) steam was generated at 3 MPa and 650 °C by recovering heat from the
 365 gasifier product gas in a high recovery steam generator (HRSG1). In IBGCC-MeOH, the surplus
 366 HP steam, after meeting the gasifier steam requirement, was used in back-pressure steam turbine
 367 ST3. In IBGCC-H₂ plant, all the steam produced in HRSG1 was used in the gasifier.

368 • In both IBGCC systems, the heat in the flue gas from the combustor (COMBUSTR, at 1200
 369 °C) was recovered into VHP steam generation in a high recovery steam generator (HRSG2). The
 370 same flue gas was further expanded in a turbo-expander (TEXP) to generate power for the air
 371 compressor (AIRCOMPR in **Fig. 5** and **Fig. 6**). Thus surplus power was generated. In the integrated
 372 biodiesel system, the VHP steam generated in HRSG2 was first used to fulfil the heat requirement
 373 by the reboiler in the biodiesel recovery column before generating power from the back-pressure
 374 steam turbine ST1 (**Fig. 8**).

375 • The surplus exothermic heat of reaction of the combustor (COMBUSTR), after meeting the
 376 heat requirements of the gasifier, was also recovered into VHP steam generation. In the IBGCC-H₂,
 377 all the VHP steam generated from COMBUSTR and HRSG2 was expanded through the back-
 378 pressure steam turbine (ST1) to an outlet pressure of 0.5 MPa for power generation since there was
 379 no demand for VHP steam in the green diesel plant.

380 • Excess heat from WGSR, SYNGCOOL and MEOHREAC (in IBGCC-MeOH plant) was
 381 suitable for MP steam generation. In the green diesel and IBGCC-H₂ integrated system, part of the
 382 MP steam generated was used in the oil preheater (RMIXHTR, **Fig. 4**) and the excess was utilised
 383 for power generation in back-pressure steam turbine (ST2). In the biodiesel and IBGCC-MeOH
 384 integrated system, all the MP steam generated was used to fulfil the heat demands by the biodiesel
 385 plant.

386 • LP steam generated after expansion of steam at higher levels was used to meet heat demands
 387 by the gas clean up and biodiesel or green diesel plants. Surplus LP steam was passed through
 388 condensing steam turbine for power generation. The condensate was returned as boiler feed water.

389 • The waste heat available in the syngas stream after heat recovery as MP steam in
 390 SYNGCOOL (in both IBGCC-H₂ and IBGCC-MeOH) and the methanol reactor product (in
 391 IBGCC-MeOH plant) was extracted to preheat the water used for steam generation.
 392 The net energy from the IBGCC-MeOH plant (including waste heat and heat and power generation
 393 for other biorefinery processes) was 0.35 PJ y⁻¹ as power, 0.16 PJ y⁻¹ as heat and 0.26 PJ y⁻¹ as
 394 methanol (HHV of 22.7 MJ kg⁻¹). Thus, the operating energy efficiency of IBGCC-MeOH plant is
 395 42.3%, based on HHV of husk. Similarly, the net energy produced from IBGCC-H₂ plant was 0.32
 396 PJ y⁻¹ as power, 0.04 PJ y⁻¹ as heat and 0.4 PJ y⁻¹, as hydrogen. Thus, the operating energy
 397 efficiency of IBGCC-H₂ plant is 41.8%.
 398 The CPE is reduced from 2.67 PJ_CPE y⁻¹ in the standalone biodiesel production system to 2.15
 399 PJ_CPE y⁻¹ in the integrated system, resulting in further CPE saving by 19%. The total GWP
 400 impact (as) is reduced from 266.9 Gg CO₂-eq y⁻¹ to 211.2 Gg CO₂-eq y⁻¹ (21% reduction) in the
 401 integrated biorefinery compared to standalone biodiesel production system. The CPE is reduced
 402 from 2.89 PJ_CPE y⁻¹ in the standalone green diesel production system to 2.15 PJ_CPE y⁻¹ in the
 403 integrated system, resulting in CPE saving by 25%. The total GWP impact (as CO₂-eq) is reduced
 404 from 258.9 Gg y⁻¹ CO₂-eq to 211.2 Gg y⁻¹ CO₂-eq (18% reduction) in the integrated biorefinery
 405 compared to standalone green diesel production system.
 406 An excess power of 0.28 PJ y⁻¹ in the biodiesel system and 0.23 PJ y⁻¹ in the green diesel system
 407 can be exported to grid. Using the system expansion approach to consider the credits from the
 408 substitution of equivalent fossil-based products (i.e. fuel oil substituted by glycerol, soy meal by
 409 seed cake and grid electricity by electricity from the biorefinery system), the net CPE and GWP
 410 savings are determined. The CPE and GWP savings from biodiesel with respect to fossil based
 411 diesel are increased to 95% and 72%. The corresponding CPE and GWP savings from green diesel
 412 with respect to diesel are increased to 92% and 70%, respectively.
 413 The integrated biorefinery systems are self-sufficient to supply energy and methanol or hydrogen by
 414 on-site production. The CPE and GWP savings are similar in both biofuel systems. There are

greater savings from replacement of methanol, and especially heat and power in the integrated biodiesel system. However, the green diesel system is more suitable for integration with crude oil-based refinery infrastructure and might receive further support especially from crude oil companies.

4.2 Alternatives for whole *Jatropha* fruit utilisation

The results of total CPE and GWP of the systems studied are shown in **Figure 9** for the functional unit of 1 MJ of biofuel energy output. The standalone plants are taken as the base case for comparison. The integrated systems (indicated as Int) correspond to the strategic integration of biofuel plants with husk utilisation in IBGCC systems. The integrated systems combined with options for the utilisation of cake, shells and glycerol are indicated as Int-1 to Int-5. The net values are the sum of the impacts incurred and the credits obtained from the exported co-products due to substitution of fossil products.

Biodiesel systems are environmentally more benign than green diesel systems. This is mainly due to the higher avoided impact from displacement of fossil-based methanol in the biodiesel plant than from fossil-based hydrogen displacement in the green diesel plant. In addition, the credits from grid electricity substitution are lower in the green diesel system due to lower electricity generation.

In Int-1, the use of cake to provide heat allowed avoiding the impacts from the use of natural gas in seed processing and diesel for seed drying (within the cultivation system), otherwise. The fruit shell as fuel in Int-2 brings the same benefits as the cake in Int-1. This allows the utilisation of the cake as fertiliser in Int-2 and as animal feed in Int-3. However, alternative 3 achieves lower GWP than Int-2 and even negative CPE, because of the substitution of soy meal by *Jatropha* cake. Int-1 to Int-3 produce the same total bioenergy output of 4.44 PJ y⁻¹ in the biodiesel system and of 4.67 PJ y⁻¹ in the green diesel system. In both biofuel systems, the CPE and GWP change from positive values to negative values when the power plant using biogas from anaerobic digestion is considered in Int-4 and 5.

Fig. 9 GWP and CPE results of biodiesel (a and b, respectively) and green diesel (c and d, respectively) in the base case (standalone plants), integrated biorefinery systems (Int) and the integrated biorefinery systems with the five alternatives (Int-1 to Int-5). BC: base case; BPP: biogas power plant; IBGCC: integrated biomass gasification and combined cycle.

443 Int-4 utilises *Jatropha* by-products (cake, shell, glycerol) to generate electricity using anaerobic
 444 digestion. The substitution of grid electricity by electricity generation using biogas resulted in
 445 further CPE savings and GWP reduction. The total bioenergy production in the biodiesel system is
 446 5.33 PJ y^{-1} while the green diesel system produces 5.71 PJ y^{-1} . However, as shown in Fig. 9, more
 447 benefits in terms of CPE and GWP savings are obtained in Int-5. Int-5 assumes that the cake is used
 448 to produce heat for oil extraction and seed drying while fruit shells and glycerol (biodiesel system)
 449 are anaerobically digested to generate electricity via biogas. In this integrated biodiesel system, 5.05
 450 PJ y^{-1} of output energy is generated in the form of biodiesel, heat and power. The total input energy
 451 is 9.45 PJ y^{-1} from *Jatropha* fruit fractions and 0.14 PJ y^{-1} from diesel used in field operations
 452 during cultivation, yielding an energy efficiency of 53%. This is an increase by 14% from the
 453 *Jatropha* oil conversion to biodiesel in the standalone (base case) process. In the green diesel
 454 system, the output energy is 5.43 PJ y^{-1} in the form of green diesel, propane fuel, heat and power
 455 output from the same total input energy as in the biodiesel system. The resulting energy efficiency
 456 is 57%. This is 16% more efficient than the *Jatropha* oil conversion to green diesel in the standalone
 457 process. The two integrated biofuel systems in Int-5 exhibit an energy yield per unit of land of 83
 458 GJ ha^{-1} . The GWP from the net bioenergy production (i.e. the energy actually exported in the form
 459 of biofuels and electricity) is $160 \text{ Gg CO}_2\text{-eq y}^{-1}$ in both systems. Thus, the average GWP per unit
 460 of bioenergy output is $29 \text{ g CO}_2\text{-eq MJ}^{-1}$. This GWP value is before accounting credits from
 461 substitution of fossil-based energy by the energy co-produced and exported from the biorefineries.
 462 After accounting for the credits from displacement of grid electricity, the CPE saving is 138% and
 463 GWP reduction is 110% in the biodiesel system, while the CPE saving is 133% and GWP reduction
 464 is 108% in the green diesel system, respectively (in Int-5). These savings are more than two-folds
 465 compared to the standalone systems. These imply that, although it might not be possible to
 466 completely de-carbonise the biofuel supply chains upstream (e.g. in the cultivation stage where
 467 extensive fertilisation is required to increase yields), the impacts can be counterbalanced by whole
 468 crop conversion into useful products in integrated biorefinery systems such as Int-5.

469 **5. Conclusions**

470 Comprehensive system modelling, simulation, integration and analysis tools have been applied to
471 generate integrated biorefinery configurations aimed at high efficiency biofuel and energy
472 productions and fossil resource saving and low global warming potential impact. The low energy
473 efficiency of the standalone biofuel systems can be improved by converting the whole fruit into
474 energy and raw material productions. The raw materials are used up by the biofuel production
475 processes. This is achieved by on-site production of heat and power, methanol or hydrogen using
476 husk gasification. The strategic utilisation of seed husk in IBGCC systems has been explored for
477 reduction in GWP and CPE. In addition, potential benefits from the use of Jatropha cake as fuel or
478 animal feed are also explored. The GWP savings are favoured by the utilisation of cake as animal
479 feed, whilst its utilisation as fuel favours CPE savings. The benefits of integration of anaerobic
480 digestion of Jatropha fruit shells, cake and/or glycerol producing biogas used for power generation
481 has also been demonstrated. Results showed that energy and GHG emissions saving could be
482 doubled in an integrated Jatropha biorefinery exploiting the whole Jatropha fruit, compared to the
483 standalone plants only converting the Jatropha oil into biofuel production.

484 The methodological contributions from this paper are heat integration, total site utility system
485 design and synergetic material product integration. These methodological contributions made in this
486 paper allowed the substitution of fossil energy and major raw materials used for the biofuel
487 production processes and thereby savings in GWP and CPE. The use of shells and glycerol for
488 electricity production via anaerobic digestion combined with any of the potential uses of cake (as
489 fuel, fertiliser, for animal feed or also as substrate for anaerobic digestion) increased the savings
490 considerably. This led to zero or even negative CPE and GWP due to significant credits obtained
491 from the substitution of fossil products by the biorefinery products. The credits achievable are more
492 than to offset the impacts by the system. The two biofuel systems studied had very similar
493 performance regarding GWP and CPE savings. The systems are evaluated for future
494 implementation by assuming optimum parameters for Jatropha cultivation and conversion

495 processes. A sensitivity analysis and the use of other allocation approaches may be needed for
496 application of the results.

497 Although integrated systems showed environmental and energetic advantages, practicality and
498 economic feasibility studies must be carried out to allow a holistic selection of the best *Jatropha*-
499 based integrated biorefinery configuration. Biofuel properties and their adaptation to existing
500 infrastructure as well as uncertainties in prices, economic incentives and policy support need to be
501 evaluated. Furthermore, the capital required to build the various processing plants might involve
502 more than one investor and might require further incentives for cooperation to operate as a whole
503 integrated system. The processing capacity scale also needs to be optimised considering the
504 previous aspects.

505

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676 **Table 1** Elemental analysis, compositions and calorific values of various *Jatropha* products

	FRUIT		SEED		KERNEL	
	Shell ^a	Seed ^{b,d}	Husk ^{c,gh}	Kernel ^{d,g}	Oil ^e	Cake ^{f,h}
Mass (%)	31.0	69.0	33.7	66.3	58.2	41.8
C	32.52	60.71	48.5	66.92	77.40	52.3
H		8.19	5.7	9.46	11.58	6.5
O		25.33	41.0	17.35	11.01	26.18
N	3.64	1.67	0.67	2.17		4.81
S	0.02	0.16	0.01	0.24		0.58
P	0.76					2.23
K	4.93					1.5
Ash	14.88	3.93	4.08	3.86		9.24
HHV (MJ kg ⁻¹) ⁱ	17.28	27.1	19.9	30.9	39.6	18.3

- 677 a. Mass fraction in the fruit calculated after [12]. P and K values are part of the ash fraction. Elemental
678 composition from [8], [18]; H and O not reported. Heating value from [8].
- 679 b. Mass fraction in the fruit calculated after [12].
- 680 c. Elemental composition from [21].
- 681 d. Elemental composition and heating value calculated by mass and energy balance, respectively.
- 682 e. Oil fraction in kernel is at an average oil extraction efficiency of 99.1% by solvent method. Efficiency derived
683 from [10]. Heating value from [5]. Elemental composition from simulation results.
- 684 f. Elemental composition determined from [15], [22]. P and K are part of the ash fraction.
- 685 g. Average mass fraction calculated from [9], [10], [11] and [13].
- 686 h. Average heating value calculated from [9], [10], [11] and [13].
- 687 i. HHV: high heating value

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Table 2 CPE and GWP factors for materials and energy used or produced in the various Jatropha subsystems

Item	Functional unit	CPE (MJ_CPE)	GWP (g CO ₂ -eq)	Reference
N fertiliser (Urea)	kg	49.25	2940	[45]
P fertiliser (Triple superphosphate)	kg	18.81	1160	[45]
K fertiliser	kg	5.6	380	[45]
Machinery (manufacturing and storage)	h	40.81	2.912	[45]
Storage buildings	m ² y	51.69	4.721	[45]
Abamectin (pesticide)	L	190	13.12	[45]
Glyphosate (herbicide)	L	190	13.12	[45]
Diesel	MJ	1.114	74.4	[46]
Electricity mix	MJ	2.597	173.4	Estimated from [50]
Natural gas (NG)	MJ	1.016	61.2	[45]
Liquefied petroleum gas (LPG)	MJ	1.06	76.4	[47]
Fuel Oil	MJ	1.11	94.9	[45]
Hexane	kg	37.5	861	[7]
Methanol	kg	12.872	2836	[33]
Hydrogen	kg	183.2	11888	[48]
Soy meal	kg	4.13	726	[49]

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706 **Table 3** Reported measured yields of *Jatropha* plantations in different locations and estimated
707 annual seed yield at maturity [12], [14], [51], [52]

Location	AAR (mm)	Age, A (y)	Reported yield at age A, Y_A (kg/ha)	Yield at maturity, Y_m (kg/ha)
Bawal, India	521	3	208	300
Jaipur, India	668	2.5	313	500
Erode, India	693	2.5	350	550
Kapiri Mposhi, Zambia	744	2.5	500	780
Nashik, India	690.5	5	1200	1200
Hyderabad, India	812.5	3	911	1400
Digini, Mali	1020	2	550	1500
Andhra Prades, India h	925	2.5	1000	1680
Surubaya, Indonesia	1751	2	1000	1950
Sinaloa, Mexico	600	2	980	1966
Tamil Nadu, India	945	3	1573	2000
Allahabad, India	998	4	2000	2300
Bhavnagar, India	800	2	1270	2400
Tirunelveli, India	736.9	3	2000	2600
Leon, Nicaragua	1593	4	2500	2750
Managua, Nicaragua	1200	4	3484	3915
Paraguay	1370	8	4000	4000
Sinaloa, Mexico	1453	2	2040	4092
Thailand	1470	1	794	5456
Maximum	1500			5000

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709 **Table 4** Inventory data for Jatropha cultivation in the location under study

Inventory	Amount input
N fertiliser	162 kg/ha
P fertiliser	162 kg/ha
K fertiliser	162 kg/ha
Machinery	2h/ha, 42.6 kW tractor
Diesel	6584 MJ/ha
Electricity from grid	27.8 MJ/ha
Storage area	3.7 m ² /ha
Abamectin (pesticide)	2 L/ha
Glyphosate (herbicide)	2 L/ha

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719 **Table 5** Specifications for the biodiesel simulation in Aspen Plus

Equipment	Model	T (°C)	P (kPa)	Other specifications		Reference
RMIXHTR	Heater	70	101.3			[6]
TEREACT	Rstoic	70	101.3	Tryglycerides conversion fraction	0.93	[6]
				Free fatty acids conversion fraction	1	Assumed
MEOHREC	RadFrac		40	Pressure drop (bar)	0.1	Assumed
				Stages	16	From simulation
				Methanol mass recovery (%)	99	Specified
				Molar reflux ratio	2	From simulation
RECPUMP	Pump		200			
COOL1	Heater	25	101.3			
DECANT	Decanter	25	101.3			
BIODREC	RadFrac		101.3	Stages	4	From simulation
				FAME mass recovery (%)	99	Specified
				Molar reflux ratio	0.2	From simulation
PREH1	Heater		101.3	Duty (MW)	2.27	From simulation
PREH1-1	Heater	35	101.3			Specified
COOL2	Heater	35	101.3			Specified

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723 **Table 6** Specifications for the green diesel simulation in Aspen Plus [7]

Equipment	Model	T (°C)	P (kPa)	Other specifications	
HE1	HeatX			Hot Stream Outlet T (°C)	275
RMIXHTR	Heater	188	3450		
H2TRECTR	RYield	325	3450	Mass yield fractions:	
				GDIESEL	0.8415
				PROPANE	0.0290
				WATER	0.0213
				CO ₂	0.1063
				H ₂	0.0020
OILPUMP	Pump		3450	Isentropic efficiency	0.85
PHASESEP	Flash2	35	1200	Free water phase valid	
PSA	Sep			Component mass split fraction:	
				CO ₂ in stream CO2	1
				PROPANE in stream CO2	0
				H ₂ in stream H2RECVD	1
				Others in stream H2RECVD	0
GDISLREC	RadFrac		101.3	Stages	8
				No condenser, no reboiler	
LPGSEP	Flash2	20	101.3	Free water phase valid	
H2FCOMPR	Compresor		3450	Isentropic efficiency	0.85
H2RCOMPR	Compresor		3450	Isentropic efficiency	0.85

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Table 7 Specifications for the simulation of husk conversion into heat, power and methanol or hydrogen via gasification

Name	Model	T (°C)	P (MPa)	Other specifications	
AIRCOMPR	Compr		3	Isentropic efficiency	0.85
MPRODEXP	Compr		4.1	Isentropic efficiency	0.9
OFFGCOMP	Compr		3	Isentropic efficiency	0.85
B1	Fsplit			Flow rate (t d ⁻¹) for steam to biomass	94.93
				ratio = 0.35 in IBGCC-MeOH	
				Mass split fraction in IBGCC-H ₂	1
B5	Flash2	55	0.1		
RECWPUMP	Pump		3	Isentropic efficiency	0.85
B19	Fsplit			Mass split fraction	0.2384
				(IBGCC-MeOH)	
COMBUSTR	RGibbs	1200	3		
CYCLONE	SSplit			Ash mass split fraction	1
EFFLUSEP	Flash2	55	3		
GCLEANUP	Sep2	55	3	CO ₂ mass split fraction	0.9
				H ₂ S and COS mass fraction	1
HRSG1	HeatX			Hot stream outlet T (°C)	450
MEOHREAC	Requil	250	10		
MEOHREC	Flash2	55	3		
STGASIFY	RGibbs	1100	3		
SYNGCOMP	Compr		10	Isentropic efficiency	0.85
SYNGCOOL	Heater	55	3		
WGSR	Requil	450	3		
PSA	Sep			H ₂ mass split fraction	0.8
			0.1	OFFGAS stream flash pressure	

746 **Table 8** LCA results for the biodiesel and green diesel standalone systems for the calculation basis
 747 of 104.7 Gg y⁻¹ of Jatropha oil and for the functional unit of 1 MJ of biofuel

	Mass flow (Gg y ⁻¹)	Energy (PJ y ⁻¹)	CPE (PJ_CPE y ⁻¹)	GWP (Gg CO ₂ - eq y ⁻¹)	CPE (MJ_CPE MJ ⁻¹)	GWP (g CO ₂ -eq MJ ⁻¹)
<i>Biodiesel system</i>						
Total before credits	100.0	3.96	2.67	266.9	0.675	67.4
Net glycerol credit	10.7	0.20	-0.23	-19.3	-0.058	-4.9
Net cake credit	75.1		-0.43	-76.4	-0.109	-19.3
Net to biodiesel			2.0	171.5	0.51	43.3
<i>Green diesel system</i>						
Total before credits	93.4	4.28	2.89	258.9	0.675	60.49
Net propane fuel credit	3.4	0.16	-0.17	-12.0	-0.040	-2.8
Net cake credit	75.1		-0.43	-76.3	-0.101	-17.8
Net to green diesel			2.29	170.6	0.53	39.9

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766 APPENDIX

767 Table 9 Mass balance of the biodiesel plant

Mass fraction	JATROOIL	METHANOL	REACMIX	TERPROD	RECMETOH	GLYCFAME	CRUDEFAME	CRUDGLYC	BIODIESEL	OILWASTE
3OLEIN	0.4500	0	0.3512	0.0246	0.1171	0.0029	0.0032	0	0.0002	0.0590
3PALMITI	0.1140	0	0.0833	0.0058	0	0.0072	0.0079	0	0.0	0.1582
3LINLEIN	0.4030	0	0.2946	0.0206	0	0.0255	0.0281	0	0.0	0.5592
3STEARIN	0.0227	0	0.0166	0.0012	0	0.0014	0.0016	0	0.0	0.0315
OLEC-01	0.0103	0	0.0075	0	0	0	0	0	0.0	0.0
M-OLEATE	0	0	0	0.3360	0	0.4149	0.4571	0	0.4769	0.0827
MPALMTTE	0	0	0	0.0779	0	0.0962	0.1060	0	0.1093	0.0423
MLINLEAT	0	0	0	0.2752	0	0.3399	0.3744	0	0.3918	0.0447
MSTEARAT	0	0	0	0.0155	0	0.0191	0.0211	0	0.0211	0.0215
METHANOL	0	1.0000	0.2466	0.1694	0.8823	0.0021	0.0006	0.0169	0.0006	0.0
GLYCEROL	0	0	0	0.0731	0	0.0903	0.0001	0.9779	0.0	0.0010
WATER	0	0	0.0001	0.0006	0.0006	0.0006	0.0001	0.0052	0.0001	0.0
Mass flow (kg h ⁻¹)	13218	1426	18081	18081	3437	14644	13293	1351	12626	667
Molar flow (kmol h ⁻¹)	15.46	44.50	155.18	155.18	95.23	59.95	44.50	15.45	43.43	1.07

769 Table 10 Mass balance of the green diesel plant

Mass fraction	JATROOIL	H2FRESH	H2TOREAC	H2TRPROD	PRODGAS	CRUDGDSL	LPSTEAM	GREENDSL	CO2	LIGHTEND	PROPANE	VENT	WATER	WATER2
3OLEIN	0.4500	0	0	0	0	0	0	0	0	0	0	0	0	0
3PALMITI	0.1140	0	0	0	0	0	0	0	0	0	0	0	0	0
3LINLEIN	0.4030	0	0	0	0	0	0	0	0	0	0	0	0	0
3STEARIN	0.0227	0	0	0	0	0	0	0	0	0	0	0	0	0
OLEC-01	0.0103	0	0	0	0	0	0	0	0	0	0	0	0	0
GDIESEL	0	0	0	0.8415	0	0.9771	0	0.9708	0	0	0	0.9686	0	0
PROPANE	0	0	0	0.0290	0.1049	0.0192	0	0	0	0.6376	0.9194	0.0307	0	0
WATER	0	0	0	0.0213	0.0029	0.0011	1.0000	0.0292	0	0.2761	0.0097	0.0007	1.0000	1.0000
CO2	0	0	0	0.1063	0.8753	0.0026	0	0	1.0000	0.0863	0.0709	0	0	0
H2	0	1.0000	1.0000	0.0020	0.0168	0	0	0	0	0	0	0	0	0
Mass flow (kg h ⁻¹)	13218	360	387	13605	1617	11717	372	11793	1415	353	429	0	271	42
Molar flow (kmol h ⁻¹)	15.46	178.35	191.85	116.32	49.76	51.52	20.65	64.08	32.15	11.20	9.87	0.00	15.05	2.32

772 **Table 11** Mass balance of husk gasification and methanol production in the IBGCC-MeOH plant

Mass fraction	CHARIN	GASIN	TARIN	2-GASPD	ASH	WGSRPROD	RECYCH2O	PURGEH2O	STEAMIN2	DRYSYN	CO2+H2S	8-CLNSYN	SYNGFUEL	SYNGAS	MEOHPROD	MOFFGAS	COMBGAS	AIRIN	14-BFW	SHEATSTM
H2O	0	0.1667	0.1428	0.1564	0	0.0498	0.9597	0.0567	0.9955	0.0065	0	0.0105	0.0105	0.0105	0.0027	0.0001	0.1304	0	1	0.9955
N2	0	0.0129	0	0.0046	0	0.0047	0	0.0007	0	0.0050	0	0.0081	0.0081	0.0081	0.0004	0.0328	0.6770	0.7671	0	0
O2	0	0	0.2983	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0205	0.2329	0	0
NO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4.56E-06	0	0	0
NO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0003	0	0	0
S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2	0	0.0033	0	0.0589	0	0.0730	0	0	0	0.0772	0	0.1253	0.1253	0.1253	0	0.1399	0	0	0	0
C	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CO	0	0.4486	0	0.6095	0	0.4539	0.0003	0.0896	0	0.4790	0	0.7776	0.7776	0.7776	0.0066	0.4805	0	0	0	0
CO2	0	0.0639	0	0.1380	0	0.4130	0.0397	0.8455	0.0045	0.4266	0.9998	0.0692	0.0692	0.0692	0.0427	0.2400	0.1718	0	0	0.0045
H2S	0	0.0002	0	0.0001	0	0.0001	0	0.0002	0	0.0001	0.0002	0	0	0	0	0	0	0	0	0
CH4	0	0.0500	0	0.0053	0	0.0055	0	0.0073	0	0.0057	0	0.0093	0.0093	0.0093	0.0031	0.0291	0	0	0	0
COS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ETHAN-01	0	0.2544	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PHENO-01	0	0	0.4879	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
METHANOL	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.9445	0.0777	0	0	0	0
ASH	0	0	0.0710	0.0272	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mass flow (kg h ⁻¹)	443	5336	5764	15056	409	14647	658	134	3956	13854	5320	8534	6500	2035	1549	485	62589	55162	5188	1891
Molar flow (kmol h ⁻¹)	36.84	215.63	129.30	953.07		953.07	35.69	3.50	218.99	913.88	120.88	793.00	603.95	189.05	48.09	47.28	2250.66	1912.00	288.00	104.69

781 **Table 12** Mass balance of husk gasification and hydrogen production in the IBGCC-H₂ plant

Mass fraction	CHARIN	GASIN	TARIN	2-GAS PDT	ASH	WGS RPROD	RECYCH2O	PURGEH2O	STEAMIN2	DRYSYNG	CO2+H2S	8-CLNSYN	SYNGFUEL	SYNGAS	HYDROGEN	OFFGAS	COMBGAS	AIRIN	14-BFW
H2O	0	0.1667	0.1428	0.2895	0	0.1465	0.9553	0.0543	0.9848	0.0064	0	0.0153	0.0153	0.0153	0	0.0183	0.1463	0	1
N2	0	0.0129	0	0.0036	0	0.0037	0	0.0004	0	0.0045	0	0.0110	0.0110	0.0110	0	0.0131	0.6845	0.7671	0
O2	0	0	0.2983	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0204	0.2329	0
NO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4.54E-06	0	0
NO	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0003	0	0
S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2	0	0.0033	0	0.0516	0	0.0695	0	0	0	0.0859	0	0.2069	0.2069	0.2069	1.0000	0.0496	0	0	0
C	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CO	0	0.4486	0	0.4278	0	0.2049	0.0001	0.0315	0	0.2515	0	0.6060	0.6060	0.6060	0	0.7263	0	0	0
CO2	0	0.0639	0	0.2045	0	0.5739	0.0445	0.9121	0.0151	0.6500	0.9999	0.1567	0.1567	0.1567	0	0.1877	0.1484	0	0
H2S	0	0.0002	0	0.0001	0	0.0001	0	0.0001	0	0.0001	0.0001	0	0	0	0	0	0	0	0
CH4	0	0.0500	0	0.0014	0	0.0015	0	0.0015	0	0.0017	0	0.0041	0.0041	0.0041	0	0.0049	0	0	0
COS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ETHAN-01	0	0.2544	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PHENO-01	0	0	0.4879	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
METHANOL	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASH	0	0	0.0710	0.0214	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mass flow (kg h ⁻¹)	443	5336	5764	19099	409	18690	2717	851	7999	15123	8848	6275	4093	2182	361	1821	58287	51931	5283
Molar flow (kmol h ⁻¹)	36.84	215.63	129.30	1180.73	0.00	1180.73	146.81	21.25	440.06	1012.67	201.05	811.61	529.39	282.23	179.19	103.04	2132.08	1800.00	293.27

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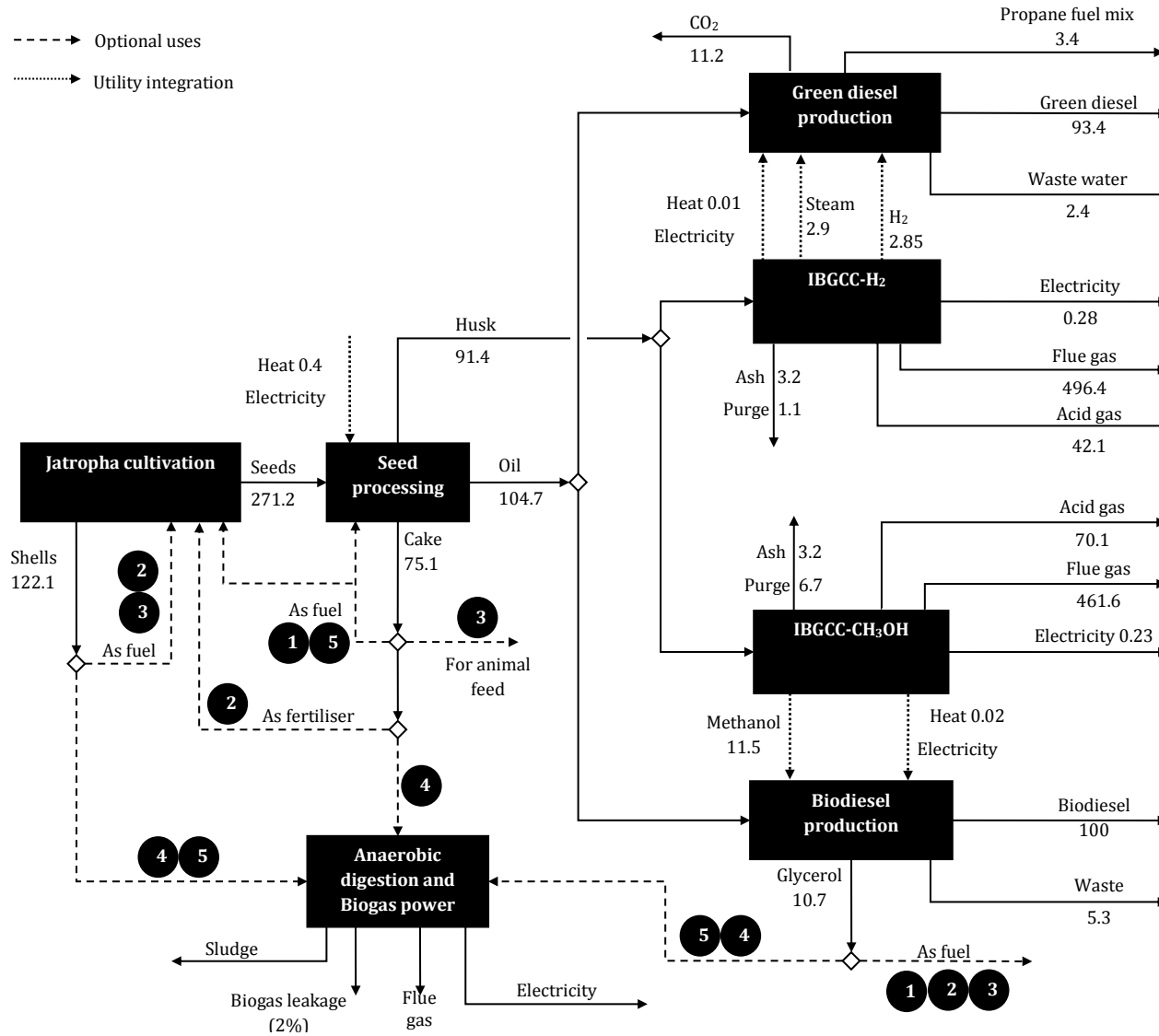
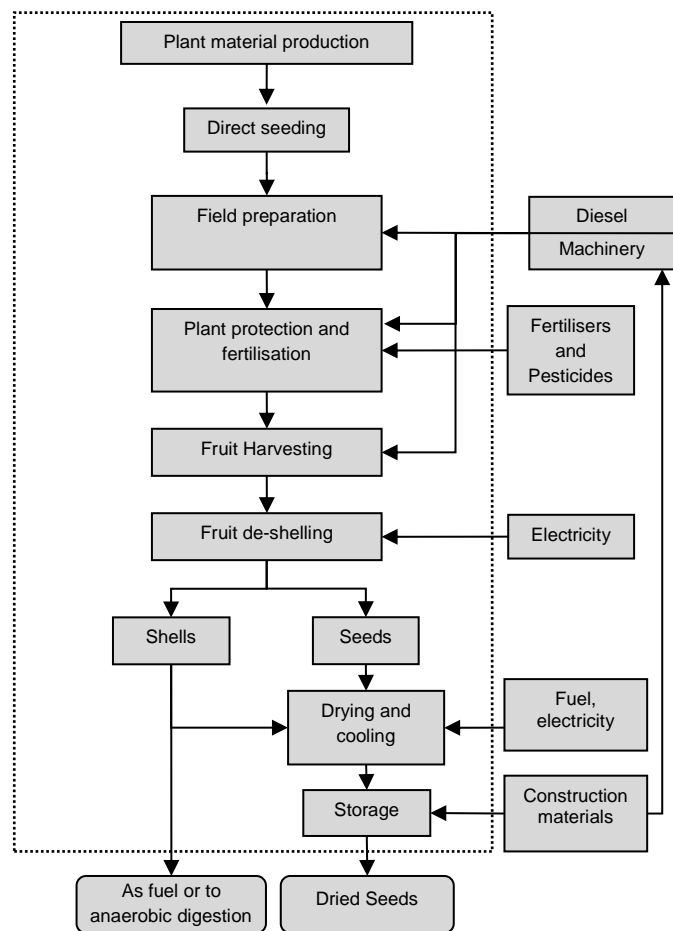


Fig. 1

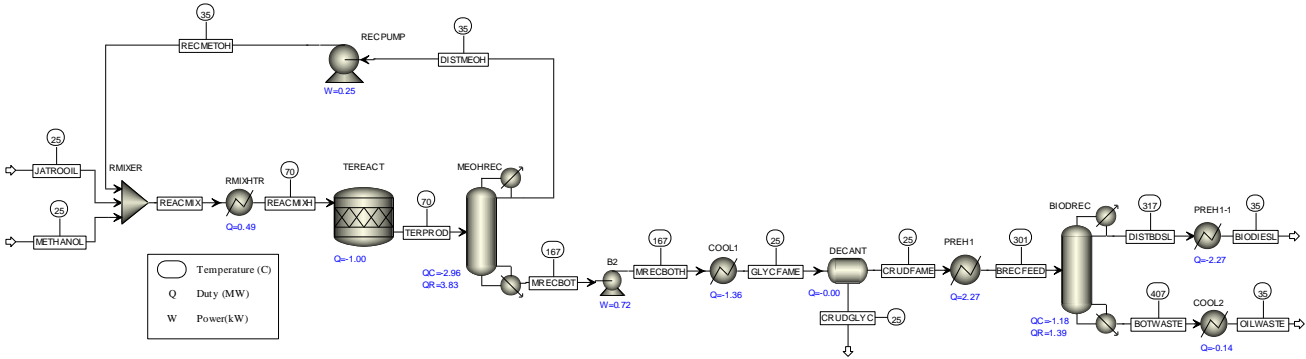


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785 Fig. 2

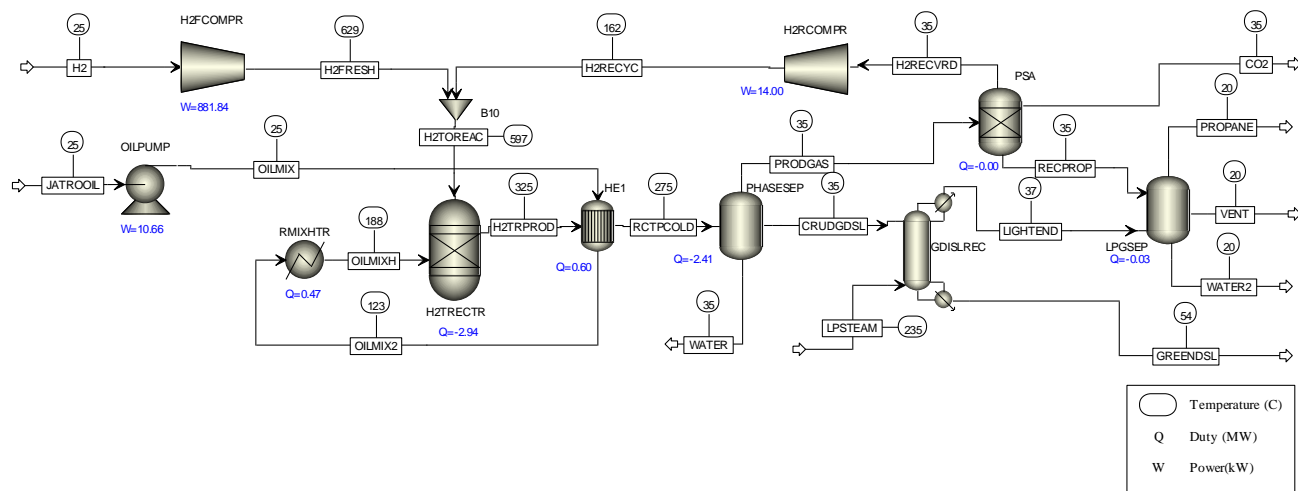
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789 Fig. 3



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791 Fig. 4

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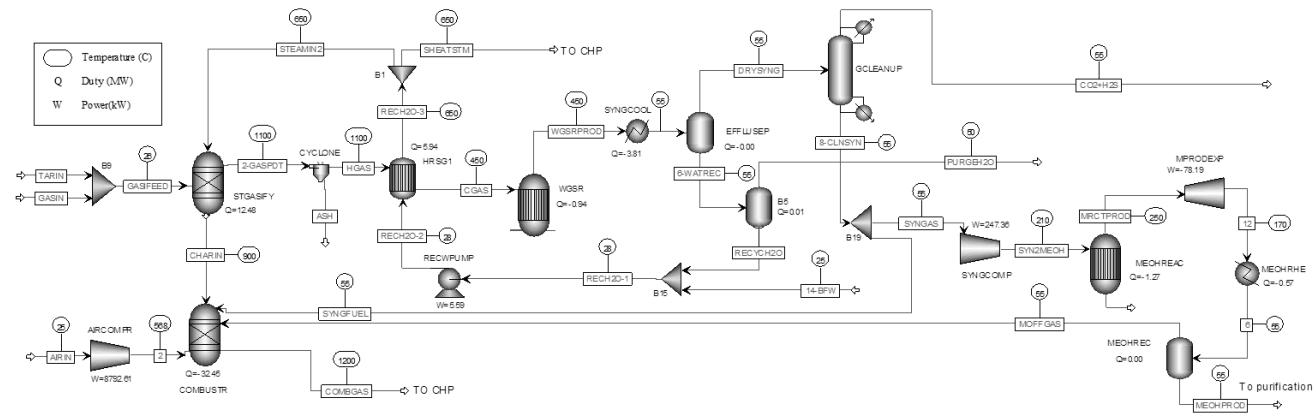


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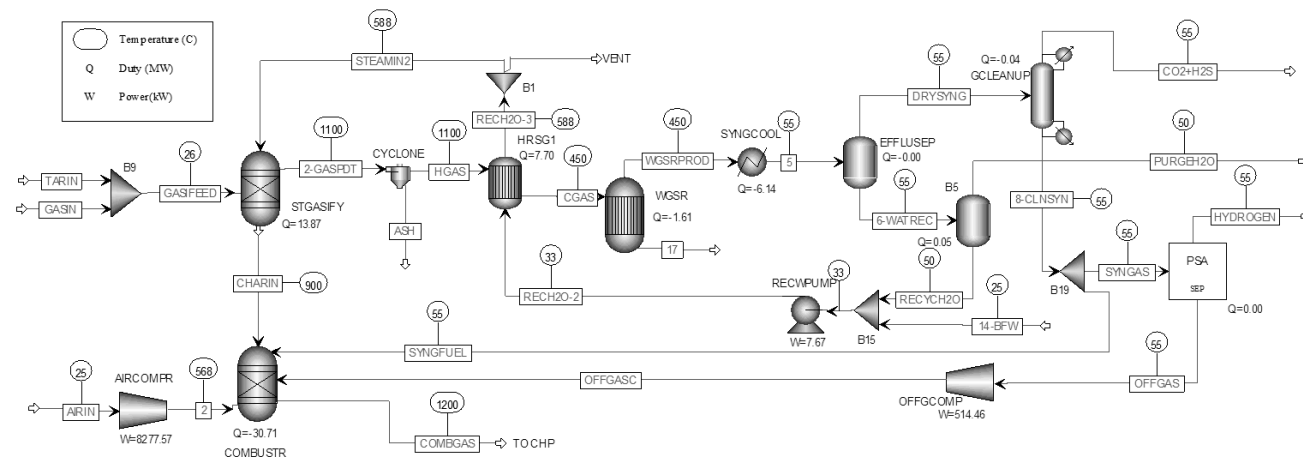


Fig. 6

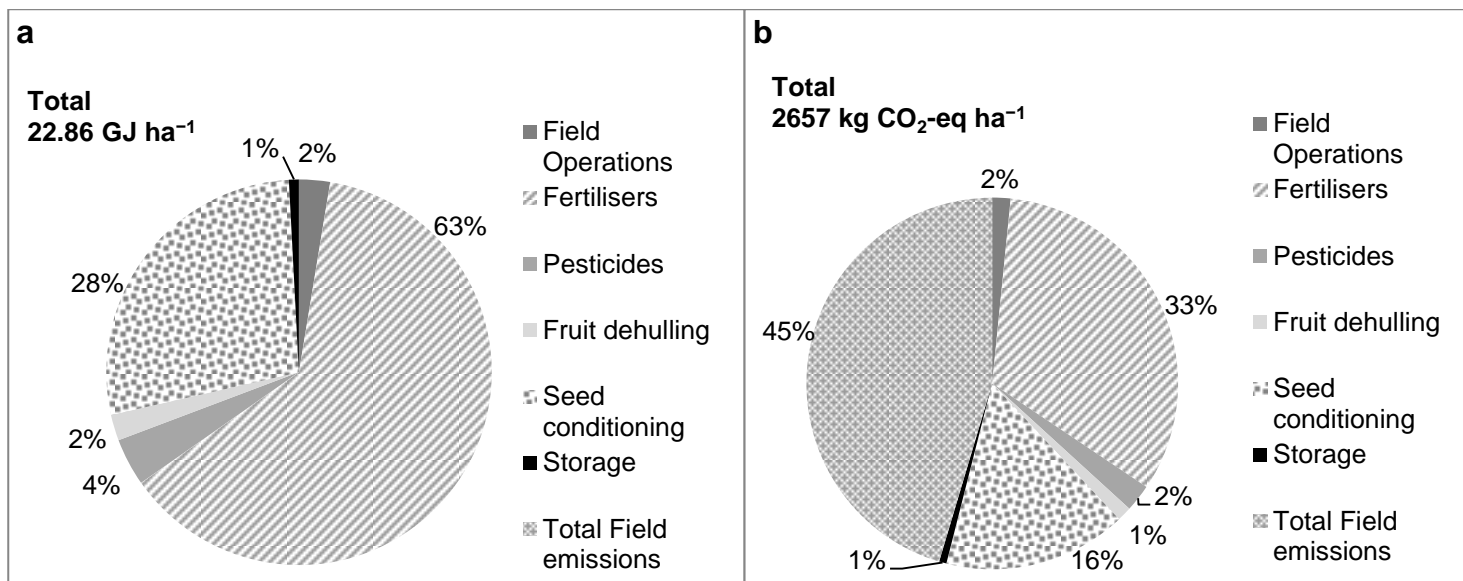
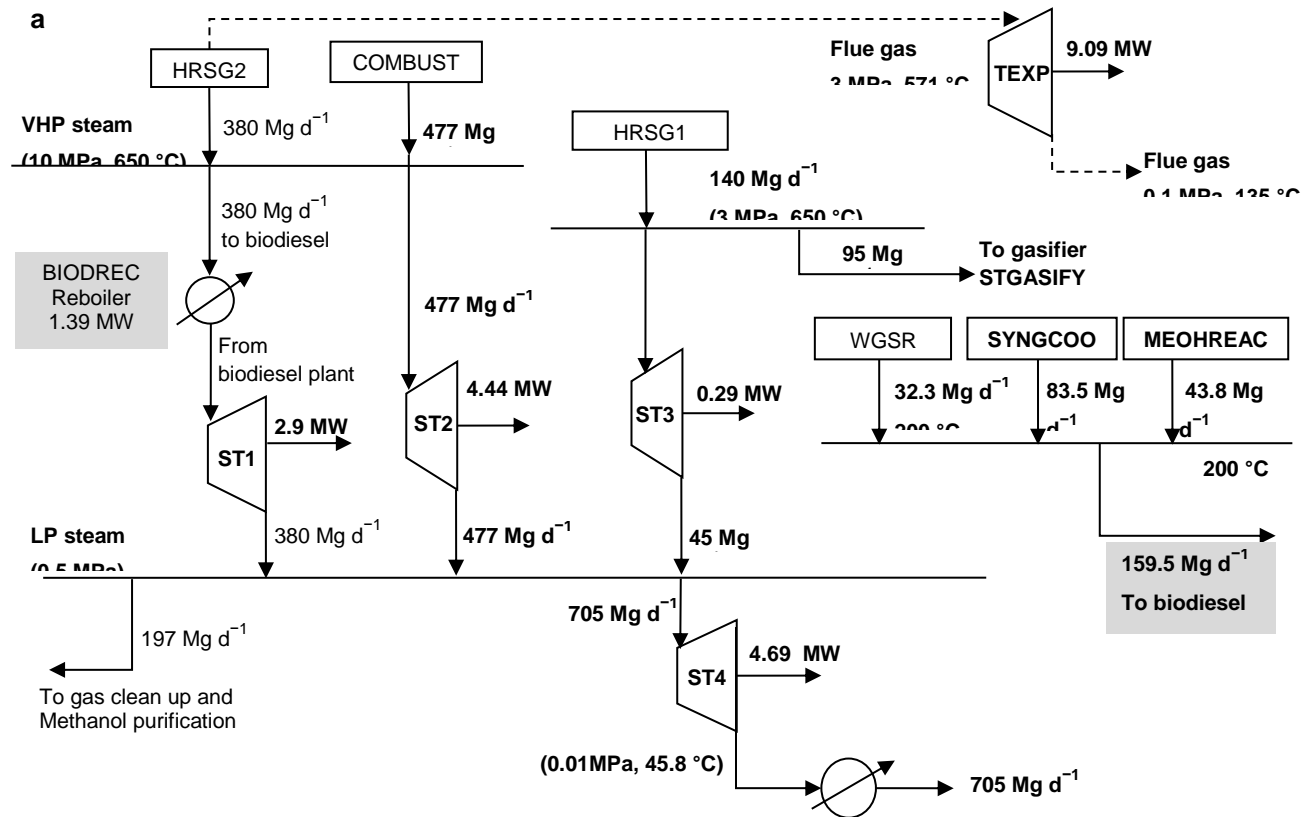


Fig. 7



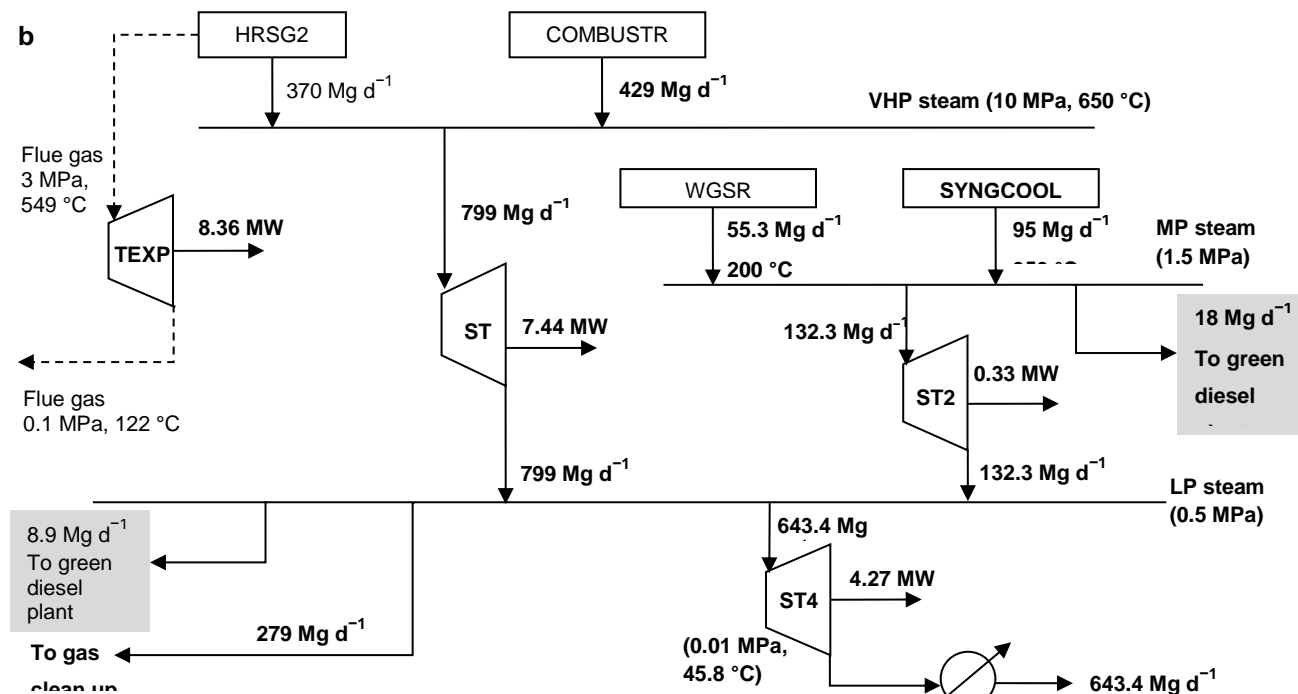


Fig. 8

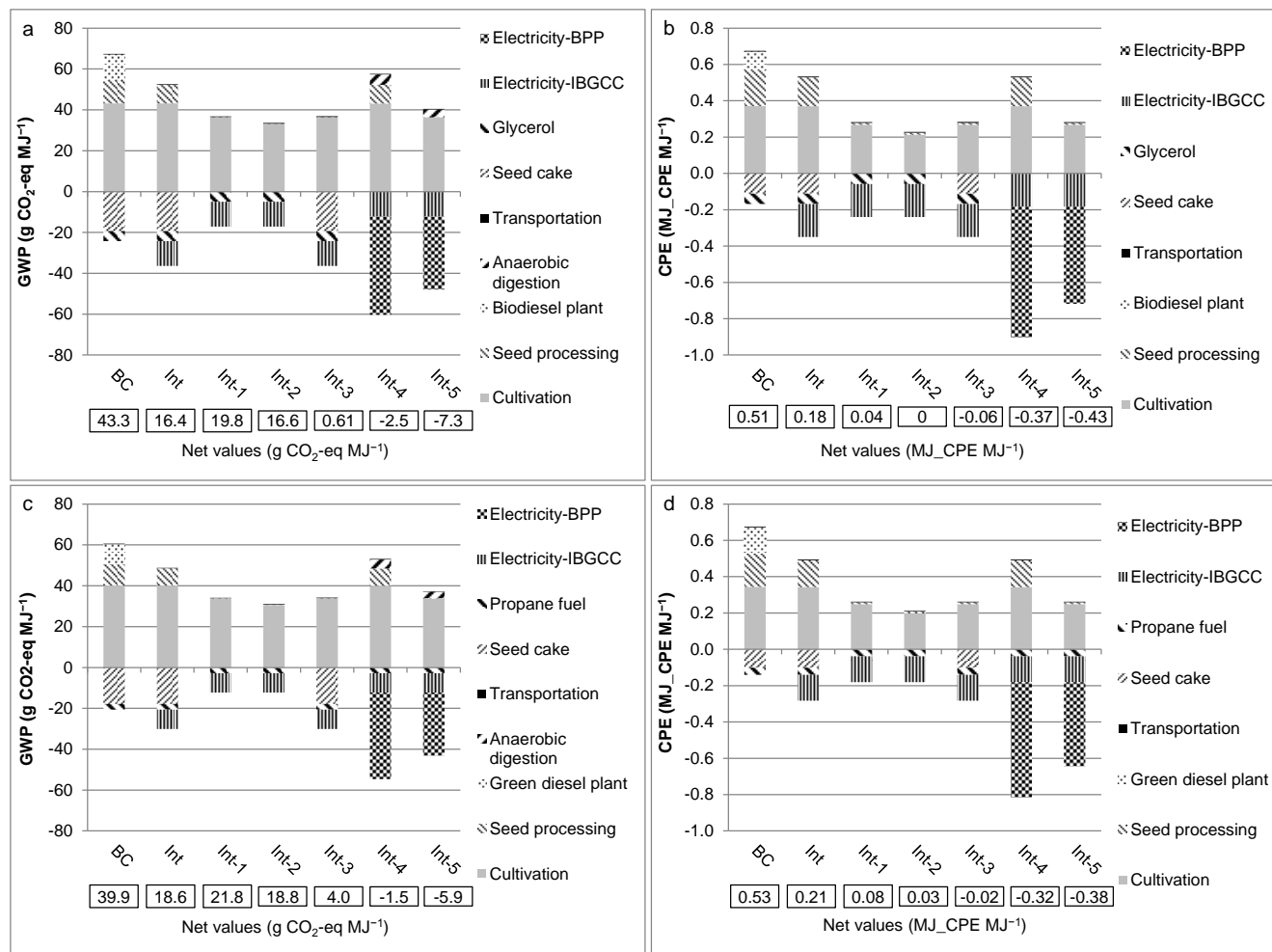


Fig. 9