Table 3.16: Results of the cogeneration model for sugarcane-bioethanol.

Parameter	Value
Q_{boiler}*	-3.007 MJ kg_{steam}^{-1}
$\Delta H_{process\ steam}$ at 12.5 bar	-2.366 MJ kg_{steam}^{-1}
$\Delta H_{process\ steam}$ at 6 bar	-2.337 MJ kg_{steam}^{-1}
$\Delta H_{process\ steam}$ at 2.5 bar	-2.297 MJ kg_{steam}^{-1}
$W_{T1\ real}$	-0.4382 MJ kg_{steam}^{-1}
$W_{T2\ real}$	-0.1327 MJ kg_{steam}^{-1}
$W_{T3\ real}$	-0.1363 MJ kg_{steam}^{-1}
$W_{T4\ real}$	-0.4044 MJ kg_{steam}^{-1}
$W_{P1\ real}$	-0.01161 MJ kg_{water}^{-1}
$W_{P2\ real}$	-0.00012 MJ kg_{water}^{-1}
Trash LHV_{AR}	-13.61 MJ kg^{-1}
Bagasse LHV_{AR}	-7.218 MJ kg^{-1}
Cellulignin LHV_{AR}	-17.44 MJ kg^{-1}

*This value is for Scenario 2.2 but will vary depending on the scenario

3.3.3 Conversion of the biomass feedstock to electricity

The conversion of the entire biomass crop (sugarcane or soybean) to electrical energy is modelled after a simple Rankine cycle as shown in Figure 3.14:

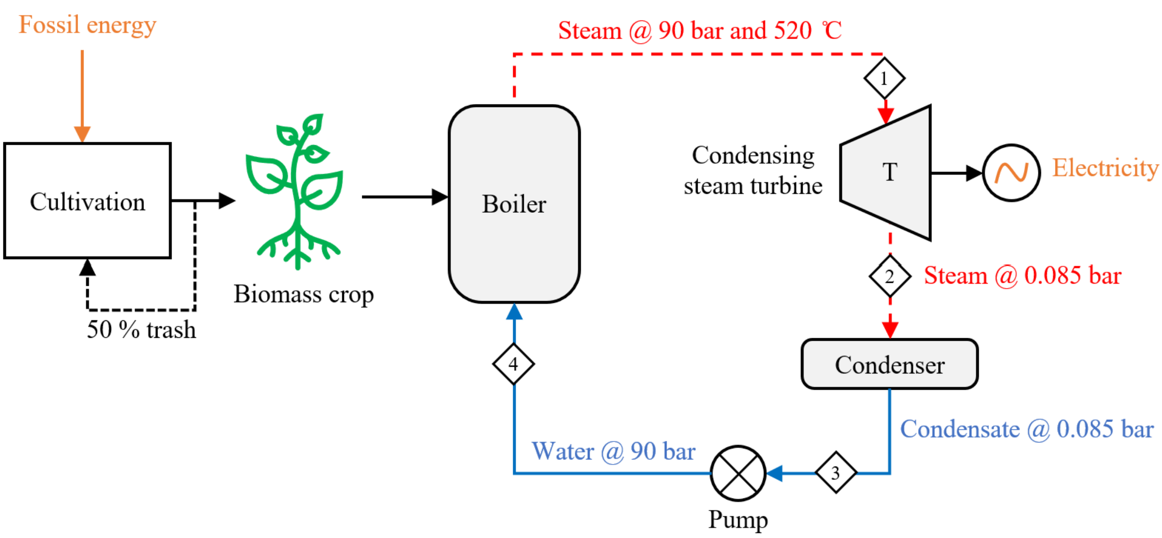

Figure 3.14: Rankine cycle for the conversion of biomass crop to electrical energy.

The steam conditions evolved from the boiler and condensing steam turbine is identical to the above cogeneration models. The condenser produces saturated water at 0.085 bar and a pump increases the water pressure to 90 bar. The conversion of the biomass crop to electricity is calculated similarly to the cogeneration model in the previous subsections. The same turbine, pump, and boiler efficiencies are used from Table 3.14. The results for the Rankine cycle model are shown in Table 3.17:

Table 3.17: Results for Rankine cycle for the direct conversion of biomass feedstock to electricity.

Parameter	Value
Q_{boiler}	-3.248 MJ kg_{steam}^{-1}
$W_{T\ real}$	-1.062 MJ kg_{steam}^{-1}
$W_{P\ real}$	-0.01134 MJ kg_{steam}^{-1}
Sugarcane Trash LHV_{AR}	-13.61 MJ kg^{-1}
Sugarcane LHV_{AR}	-2.421 MJ kg^{-1}
Soybean Trash LHV_{AR}	-14.78 MJ kg^{-1}
Soybean LHV_{AR}	-14.96 MJ kg^{-1}

3.4 The tank-to wheel cycle

After converting the biomass plant to the biofuel, the conversion of the fuel to mechanical energy in an internal-combustion engine (ICE) is modelled. This is known as the tank-to-wheel (TTW) cycle. The TTW phase measures energy consumed to supply a vehicle with energy via a pump/electric charging station to complete a driving cycle (Brito *et al*, 2013). For electric vehicles, stored electric energy is lost during the transfer of electrical energy from the charging station to the car-battery. However, for ICEs, the conservation of liquid fuels is considered to be 100 % where practically no liquid fuel losses occur.

During fuel combustion in the engine, the efficiency of converting the liquid fuel to useful mechanical energy depends on the type of engine (spark ignition for gasoline *vs.* compression ignition for diesel) and the region of the engine map at which the vehicle is operated (Brito *et al*, 2013). However, it is well established that ICEs on average only convert about 12 %–25 % of the available liquid fuel energy to useful mechanical work (Williamson, Lukic & Emadi, 2006; Leach *et al*, 2020). The upper efficiency limit of 25 % is assumed for the TTW phase, regardless of the fuel type (biodiesel *vs.* gasoline). The TTW efficiency describes that for every 100 MJ of fuel consumed by a vehicle, 25 MJ is converted into mechanical work.

Chapter 4: Methods

4.1 The system boundary

The system boundary considered in this study is shown below:

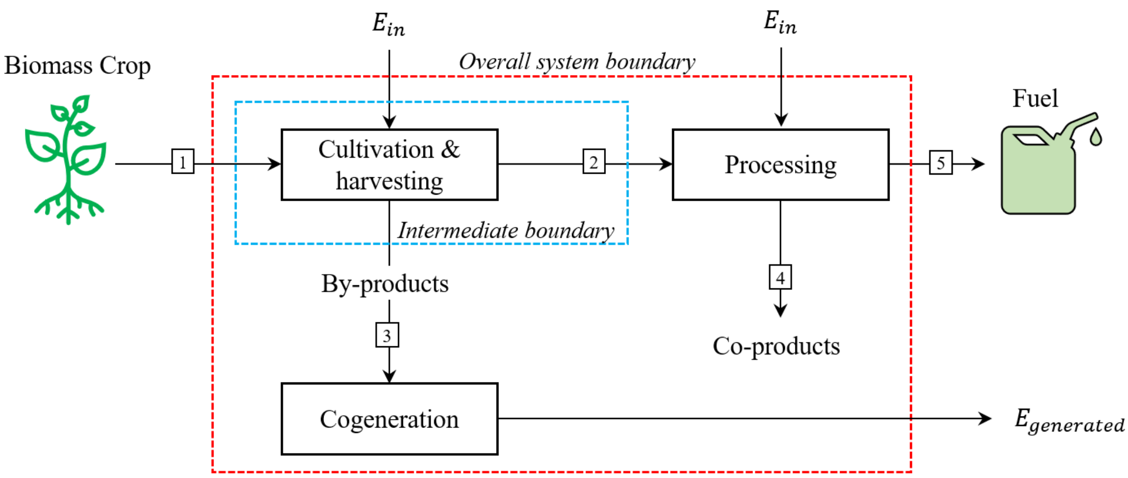

Figure 4.1: The system boundary used for this study. *The example intermediate boundary is included to illustrate the application of the energy metrics on a cumulative basis.*

The system boundary is intended to take into account *processing operations*. This is to place a focus on process efficiency rather than "life-cycle efficiency". When the boundary is extended to take into account transportation and other activities, the cross-field comparisons among biofuels becomes convoluted.

The system boundary considers the following:

- The input into the process is the entire cultivated crop. This reference state is chosen so as to embody the entire process cycle of the parent biomass.
- The energy inputs, E_{in}, considers all material and fuel inputs with an inherent higher heating value (such as diesel, natural gas, petroleum, hexane, methane etc.) and all energy utilities (such as steam and electricity). The energy consumption of the material/fuel inputs is calculated from the product of the mass flowrate and the HHV of the input. Therefore, material inputs with no calorific value are not taken into account for the energy consumption of the process.

- The system boundary is only concerned with processing operations. For this reason, the transportation of raw and intermediate products between different refineries are not considered. The only "transport energy" taken into account is for field-operations (such as diesel consumed for harvesters) as these are seen to be part of processing the biomass.

- Allocation methods are not applied. The by- and co-products are investigated in terms of their potential to improve the energy metrics; either through conversion to biofuels or to produce process heat and electricity.

4.2 Higher and lower heating values

The change in energy quality and the change in energy yield are calculated based on the energy carrying components on a dry and ash free (daf). Consequently, the energy carrying components on a daf are the components of interest for the subsequent energy metrics. Conventionally, the lower heating value (LHV) is calculated from the higher heating value (HHV) on a dry basis and considers the energy consumed to evaporate the water resulting from the combustion of fuel-bound hydrogen. The foundations of the paper rely on the strong correlation between $\Delta_c h^{\circ}{}_{\mathrm{HHV}}$ and the mass of oxygen combusted per mass of the fuel, $m_{\mathrm{O_2}}$, as described by Equation 2.3. The equation may be rewritten in terms of the elemental composition of the fuel, according to Equation 4.1 (Merckel, Labuschagne, *et al*, 2020):

$$\Delta_c h^{\circ}{}_{\mathrm{HHV}} = -13.87(n_{\mathrm{v_C}} + \frac{1}{4}n_{\mathrm{v_H}} - \frac{1}{2}n_{\mathrm{v_O}} + n_{\mathrm{v_S}} + \frac{5}{4}n_{\mathrm{v_P}})\frac{M_{\mathrm{O_2}}}{M_{\mathrm{fuel}}} \tag{4.1}$$

where $n_{\mathrm{v_C}}$, $n_{\mathrm{v_H}}$, $n_{\mathrm{v_O}}$, $n_{\mathrm{v_S}}$, and $n_{\mathrm{v_P}}$ are the moles of carbon, hydrogen, oxygen, sulphur, and phosphorus in the fuel, and $M_{\mathrm{O_2}}$ and M_{fuel} are the molar masses of oxygen and the fuel consumed during combustion respectively.

Equation 4.1 is employed to calculate $\Delta_c h^{\circ}{}_{\mathrm{HHV}}$ of the streams in the mass and energy balances and consequently, the energy metrics. However, when considering the actual energy evolved during a combustion process, the LHV, on an "as received basis" (AR), is more relevant. The LHV is calculated from the HHV by:

$$\mathrm{LHV_{daf}} = \mathrm{HHV_{daf}} - \Delta\mathrm{H_{vap}}\left(\frac{m_{\mathrm{H_2O}}}{m_{\mathrm{fuel}}}\right) \tag{4.2}$$

where ΔH_{vap} is the heat of vaporisation of water given as -2256.4 kJ kg^{-1}, m_{H_2O} is the mass of water produced during combustion of the dry fuel, and m_{fuel} is the mass of the fuel on a dry and ash free basis. The LHV_{AR} is then calculated:

$$\mathrm{LHV_{AR}} = \frac{\mathrm{LHV_{daf}}(m_{\mathrm{fuel}}) - \Delta\mathrm{H_{vap}}(m_{\mathrm{moisture}})}{m_{\mathrm{fuel_{AR}}}} \tag{4.3}$$

where m_{moisture} is the mass of moisture in the material stream and $m_{\mathrm{fuel_{AR}}}$ is the mass of the fuel on an as received basis.

The LHV_{AR} takes into account the energy consumed to evaporate the moisture in the fuel per total unit mass of the fuel (including the mass of moisture and ash-forming minerals). Therefore, the moisture and ash is only considered for the purpose of determining the LHV_{AR} of a material stream when appropriate—namely, when determining the quantity of energy evolved per unit mass of fuel during combustion with respect to a boiler.

4.3 The application of the change in energy quality

The change in energy quality, ΔE_{Q}, is applied to the system boundary according to Equation 2.4. For the biomass-to-biofuel processes, ΔE_{Q} is applied on a cumulative basis and on an overall basis. Evaluating the processing operations on a cumulative basis allows for the assessment of each unit operation.

ΔE_{Q} evaluates if the energy density of the fuel has been increased relative to the feedstock. Consequently, ΔE_{Q} only considers the material that contributes to the production of the biofuel. When applying the metric on a cumulative basis, the co-products and by-products are only taken into account if they are utilised for biofuel production. Furthermore, the energy consumed by the process is also not considered in ΔE_{Q}. For the example system boundary in Figure 4.1, the co-products are recovered as value-added products (not biofuels) and the by-products are used to generate process energy (heat and electricity). Therefore, ΔE_{Q} is computed for the intermediate boundary as

$$\Delta E_{\mathrm{Q}} = \frac{\Delta_c h^\circ|_{\mathrm{HHV},2} - \Delta_c h^\circ|_{\mathrm{HHV},1}}{\Delta_c h^\circ|_{\mathrm{HHV},1}}$$

and for the overall process:

$$\Delta E_{\mathrm{Q}} = \frac{\Delta_c h^\circ|_{\mathrm{HHV},5} - \Delta_c h^\circ|_{\mathrm{HHV},1}}{\Delta_c h^\circ|_{\mathrm{HHV},1}}$$

4.4 The application of the change in energy yield

ΔE_η, accounts for all streams that contribute to the energy recovered in the biofuel as well as for process energy. ΔE_η also considers the additional utility requirements, E_{in}, per unit of feedstock-derived energy, ΔE_{f}. In this way, ΔE_η considers the "net energy produced" during the process in relation to the biomass input.

The net energy consumed, $E_{cons.}$, is taken into account in Equation 2.6:

$$\Delta E_\eta = \frac{\Delta E_{\text{p}}}{\Delta E_{\text{f}}} - \frac{\Delta E_{\text{cons.}}}{\Delta E_{\text{f}}}$$

$$\Delta E_\eta = \frac{m_{\text{p}}\left(\Delta_c h^\circ|_{\text{HHV,p}}\right)}{m_{\text{f}}\left(\Delta_c h^\circ|_{\text{HHV,f}}\right)} - \frac{\Delta E_{\text{cons.}}}{m_{\text{f}}\left(\Delta_c h^\circ|_{\text{HHV,f}}\right)}$$

$$\Delta E_\eta = \eta\left(\frac{\Delta_c h^\circ|_{\text{HHV,p}} - \Delta E_{\text{cons.}}/m_{\text{p}}}{\Delta_c h^\circ|_{\text{HHV,f}}}\right) \tag{4.4}$$

where $\Delta E_{\text{cons.}}/m_{\text{p}}$ describes the net energy consumed per quantity of biofuel produced. It is important to note that the energy yield is normalized to the energy of the biomass into the process.

To illustrate the application of Equation 4.4, ΔE_η is defined for the intermediate boundary of Figure 4.1:

$$\Delta E_\eta = \frac{m_2 + m_3}{m_1}\left(\frac{\Delta_c h^\circ|_{\text{HHV,2}-3} - \Delta E_{\text{cons.}}/m_1}{\Delta_c h^\circ|_{\text{HHV,1}}}\right)$$

where $\Delta_c h^\circ|_{\text{HHV,2}-3}$ is the higher heating value of stream 2 and 3 combined. ΔE_η is written for the overall boundary as:

$$\Delta E_\eta = \frac{m_5}{m_1}\left(\frac{\Delta_c h^\circ|_{\text{HHV,5}} - \Delta E_{\text{cons.}}/m_1}{\Delta_c h^\circ|_{\text{HHV,1}}}\right)$$

4.5 The fossil energy ratio and net energy ratio

The fossil energy ratio (FER) and the net energy ratio (NER) for the biofuel production processes are also determined as a point of reference for the aforementioned energy metrics. The FER and NER are by no means the focus of this study. Rather, they provide insight into the current state of energy-analysis for biofuel production studies, against which the ΔE_{Q} and ΔE_{η} may be compared.

Allocation methods are not applied for the calculation of these metrics. It would be inconsistent to apply mass or energy allocation for the FER and the NER and not the ΔE_{Q} and ΔE_{η}.

The definition for the NER and FER were modified from Castineiras Filho & Pradelle (2020). The FER is given by Equation 4.5:

$$\mathrm{FER} = \frac{E_{\mathrm{surplus}} + (m_p)\Delta_c h^{\circ}|_{\mathrm{HHV,p}}}{E_{\mathrm{fossil}}} \tag{4.5}$$

where E_{surplus} is the energy of the surplus electricity produced, E_{fossil} is the fossil-derived energy consumed, and m_p is the mass of the biofuel, or product. Equation 4.5 therefore describes the total energy produced in the form of electricity and the biofuel relative to the fossil fuel energy consumed.

The NER, given by Equation 4.6, is similar to the FER. However, energy derived from renewable biomass (namely during cogeneration) is taken into account in the denominator:

$$\mathrm{NER} = \frac{E_{\mathrm{surplus}} + (m_p)\Delta_c h^{\circ}|_{\mathrm{HHV,p}}}{E_{\mathrm{fossil}} + (m_{\mathrm{biomass}})\Delta_c h^{\circ}|_{\mathrm{HHV,biomass}}} \tag{4.6}$$

where m_{biomass} and $\Delta_c h^{\circ}|_{\mathrm{HHV,biomass}}$ are the mass and higher heating value of biomass respectively. The biomass considered in Equation 4.6 refers only to biomass utilised for process steam and electricity. It does not refer to the feedstock crop which is the input into the process. This is inline with the way in which the NER is applied in life-cycle assessment studies.

4.6 Scenario definition

4.6.1 Biodiesel scenarios

Four groups of scenarios are modelled to for the soybean-biodiesel (SBD) process (see Figure 4.2):

- Scenario 1 is the ideal valorisation of the entire soybean crop. Scenario 1 is a theoretical maximum against which the real-life scenarios may be compared. The ideal valorisation considers the valorisation of the entire soybean crop including all trash that is produced. Where the real cultivation of soybean includes recycling of 50 % of the trash, this scenario includes 100 % of the trash for upgradation. The recycling of 50 % trash for fertilisation is a real-process parameter that hinders the energy recovery of the crop.

Group 2 are the upgradation scenarios of the soybean crop to biodiesel in a realistic refinery:

- Scenario 2.1 represents a production plant where no biomass is combusted for process steam and electricity—these energy inputs are derived from fossil fuel only.
- Scenario 2.2 considers the combustion of all of the available trash for cogeneration (50 % retrieved from the field where the remaining 50 % is used as a fertiliser).
- Scenario 2.3 considers the maximum production of surplus electricity, where all of the by-products and co-products are sent to cogeneration (including soybean hulls, meal, glycerol, and available trash).

Scenario 3 and Scenario 4 represent the end-use of the soybean biodiesel and plant respectively:

- Scenario 3 considers that the biodiesel produced is used in an internal combustion engine and converted to mechanical energy—this is the predominant intended end-use of liquid biofuels. Scenario 3 is based on Scenario 2.2 because this is representative of the operation of a realistic plant, where the co-products (meal, hulls, and glycerol) are sold in separate markets to maximise economic feasibility and only the waste soybean trash is burnt for process steam and electricity.
- Scenario 4 is where no valorisation of the soybean crop to biodiesel occurs, but where the entire available crop is burnt to generate electricity.

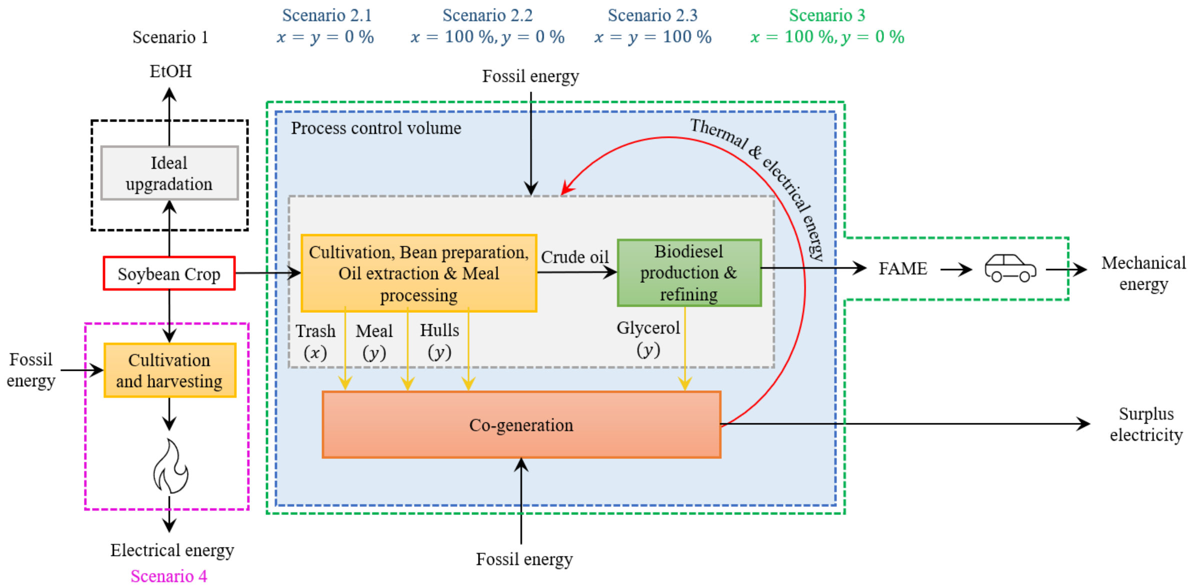

Figure 4.2: Summary of the scenarios evaluated for biodiesel production.

4.6.2 Bioethanol scenarios

As with the soybean model, four groups of Scenarios are evaluated for the sugarcane-bioethanol (SBE) process (see Figure 4.3 for reference):

- Scenario 1 represents the ideal upgradation of sugarcane to bioethanol.

Group 2 are real scenarios that focus on the production of bioethanol and the amount of excess electricity that may be produced.

Group 2A for bioethanol is intended to compare the energy metrics of the standalone 1G and 2G processes, and the integrated 1G-2G model without any energy recovery from the lignocellulose by-products:

- Scenario 2-1G is the 1G bioethanol process without the cogeneration of trash or bagasse.
- Scenario 2-2G is the standalone 2G process without cogeneration of lignocellulose.
- Scenario 2-1G2G is the integrated 1G and 2G process without cogeneration of lignocellulose.

Group 2B evaluates a more optimised bioethanol plant. Cogeneration of lignocellulose is considered and the model parameters are varied to evaluate the optimal configuration of converting the lignocellulose to bioethanol *vs.* process steam and electricity:

- Scenario 2.1 represents the 1G bioethanol production where all of the available trash and bagasse are used to generate process steam and electricity. This is representative of traditional bioethanol facilities that combust the lignocellulosic material in cogeneration.
- Scenario 2.2 is the integrated 1G and 2G facility that is at the point of energy self-sufficiency. Just enough trash and bagasse is burnt to replace the fossil fuels required by the boiler.
- Scenario 2.3 considers the maximum bioethanol production in a realistic scenario. All of the trash and bagasse are valorised to bioethanol in the integrated 1G and 2G process. The only lignocellulose sent to cogeneration is the cellulignin (a by-product of the 2G process). Therefore, fossil fuels are required for the boilers to supplement the process energy requirements.

Groups 3 and 4 take into account the end-use of the biofuel or the initial biomass crop:

- Scenario 3 is based on the parameters of Scenario 2.2— the 1G and 2G energy autonomous process. This scenario is intended to evaluate the use of bioethanol in an internal combustion engine to represent the end-use of the fuel.
- Scenario 4 assesses the conversion of the biomass crop directly to electricial energy, where no biofuel is produced. This scenario is intended to represent a theoretical end-use of the biomass crop.

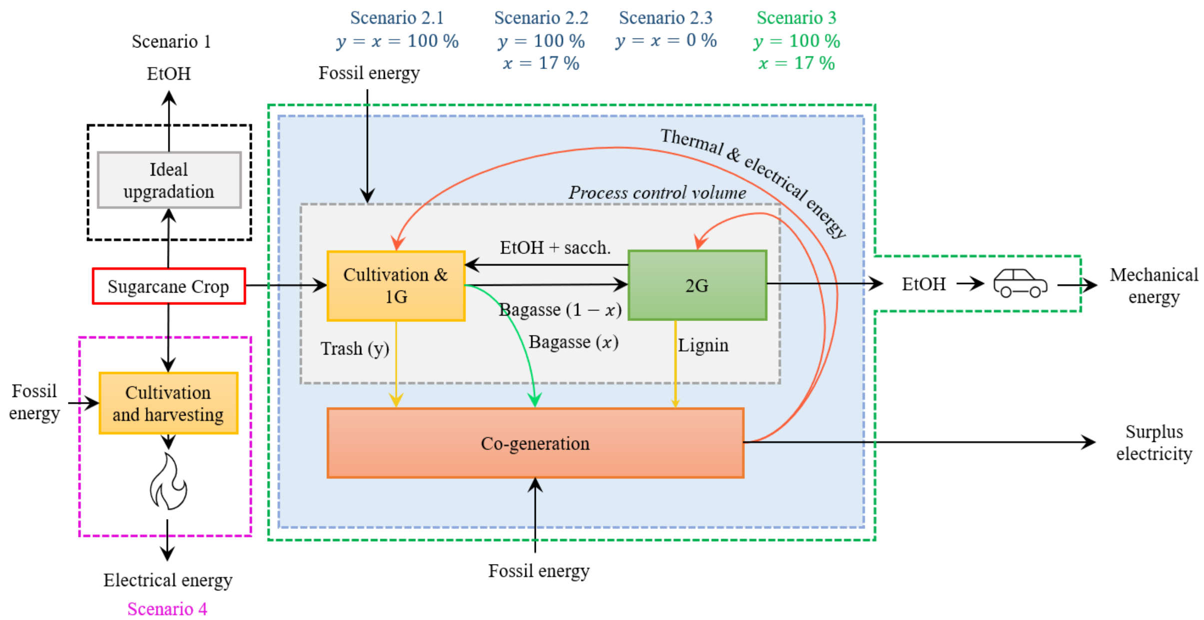

Figure 4.3: Summary of the scenarios evaluated for bioethanol production.

Chapter 5: Results and discussion

5.1 Ideal conversion of biomass to biofuels (Scenario 1)

The theoretical upgradation of the cultivated sugarcane and soybean crop is illustrated in Figure 5.1. The ternary diagram shows the hypothetical maximum mass yield for the biomass-to-biofuel conversion, and the average composition of the waste products. The mass yield (η), and consequently, the change in energy quality (ΔE_Q) and the change in energy yield (ΔE_η) are calculated from the tie lines. For this exercise, the entire crop is taken as the input for the ideal conversion process. This includes all of the trash. The trash left on the field after harvesting (50 wt. %) is considered as a real process parameter.

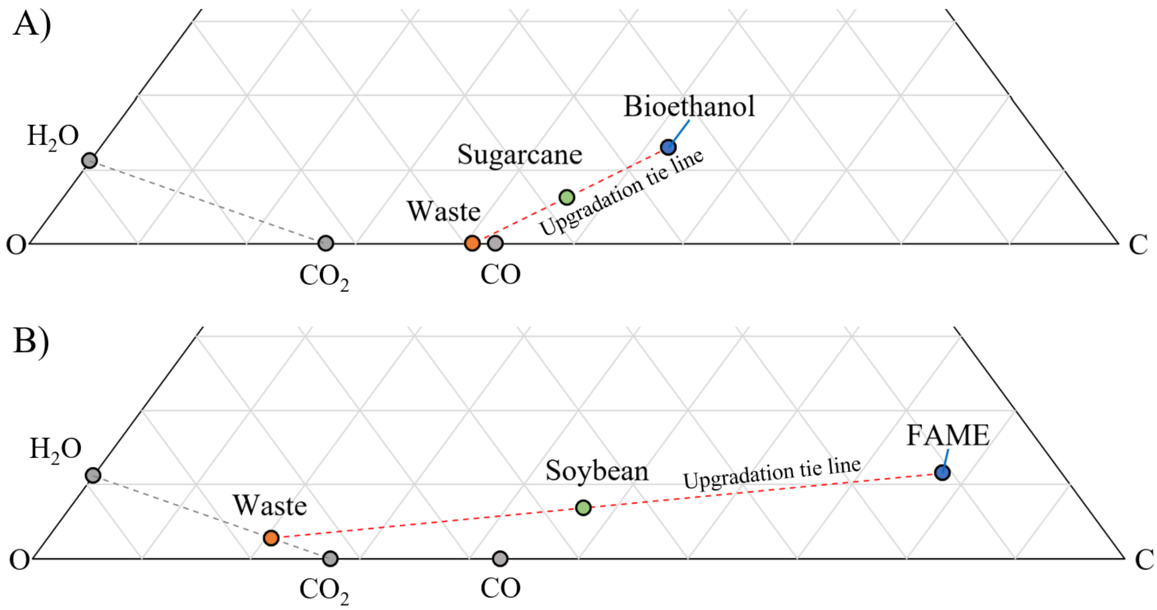

Figure 5.1: Ternary diagram showing the ideal conversion of the sugarcane crop to bioethanol (A) and the soybean crop to FAME (B). *The compositions are plotted on a mass and daf basis.*

The waste products/upgradation losses do not represent a single compound. Rather, the upgradation losses represent the minimum loss of energy-containing carbon and hydrogen in order achieve the maximum mass yield of the biofuel from the biomass:

- The sugarcane crop may undergo decarbonylation and decarboxylation to produce bioethanol, where CO and CO_2 are removed from the feedstock respectively.

- The soybean crop may undergo decarboxylation and dehydration to produce biodisel, where CO_2 and H_2O are removed from the feedstock respectively.

Table 5.1 indicates the mass compositions of the feedstock and products, as well as the theoretical mass yield, change in energy quality, and change in energy yield.

Table 5.1: Results from the ideal valorisation of the soybean and sugarcane plant. *The upgradation losses are a combination of H_2O, CO_2, CO, or C.*

Component	C (wt. %)	H (wt. %)	O (wt. %)	η (%)	ΔE_Q (%)	ΔE_η (%)
Soybean crop	47	7	46	-	-	-
FAME	78	12	11	47	107	97
Upgradation losses	20	3	77	53	-100	0
Sugarcane crop	46	6	47	-	-	-
Bioethanol	52	13	35	48	63	79
Upgradation losses	41	0	59	52	-100	0

The removal of oxygen in the form of water, carbon dioxide, and/or carbon monoxide results in an increase in the oxidation potential of the product from the feed $\left(\frac{m_{O_2|p}}{m_{O_2|f}} > 1\right)$, and therefore, the energy quality increases. The removal of oxygen from the feed in the form of CO_2 is preferred; when the goal is to increase energy density, H/C ratio should be maximised.

Even though the theoretical maximum for η for the biofuels is 47 %–48 %, the ΔE_Q and ΔE_η achieved is relatively high. This is because the higher heating value (HHV) of the biofuel is greater than that of the feed:

- For FAME, the ΔE_Q is 107 %. This is due to the fact that the HHV of biodiesel is more than double that of the feed (-40 MJ kg^{-1} *vs.* -19 MJ kg^{-1}). The ΔE_η is also high (97 %). This is as a result of Equation 2.7 which shows that ΔE_η is a function of the mass yield and the change in energy quality. Theoretically, almost all of the original energy contained in the soybean feedstock can be recovered in biodiesel.

- For bioethanol, the ΔE_Q is 63 %. The change in energy quality for bioethanol is much lower than that of biodiesel due to the lower HHV of bioethanol (-29 MJ kg^{-1}) *vs.* biodiesel (-40 MJ kg^{-1}). The ΔE_η for bioethanol production (79 %) is lower than that of biodiesel production for the same reason.

The ideal conversion results are used as baseline against which the real scenarios are compared.

5.2 Evaluating the configurations of biodiesel production (Scenarios 2.1–2.3)

5.2.1 The cumulative ΔE_Q and η for soybean to biodiesel production

The change in energy quality, ΔE_Q, *vs.* the mass yield yield, η, for the biodiesel production process (Scenarios 2.1–2.3) is shown in Figure 5.2 and Table 5.2. The change in energy quality has been defined in such a way so as to only consider the recoverable material streams that contribute to the production of the biofuel. ΔE_Q communicates whether the feedstock has been upgraded into a more energy dense carrier. The difference among Scenarios 2.1, 2.2, and 2.3 is merely the diversion of the waste/co-products to cogeneration which has no effect on the biodiesel yield. Hence, all 3 scenarios achieve the same plot.

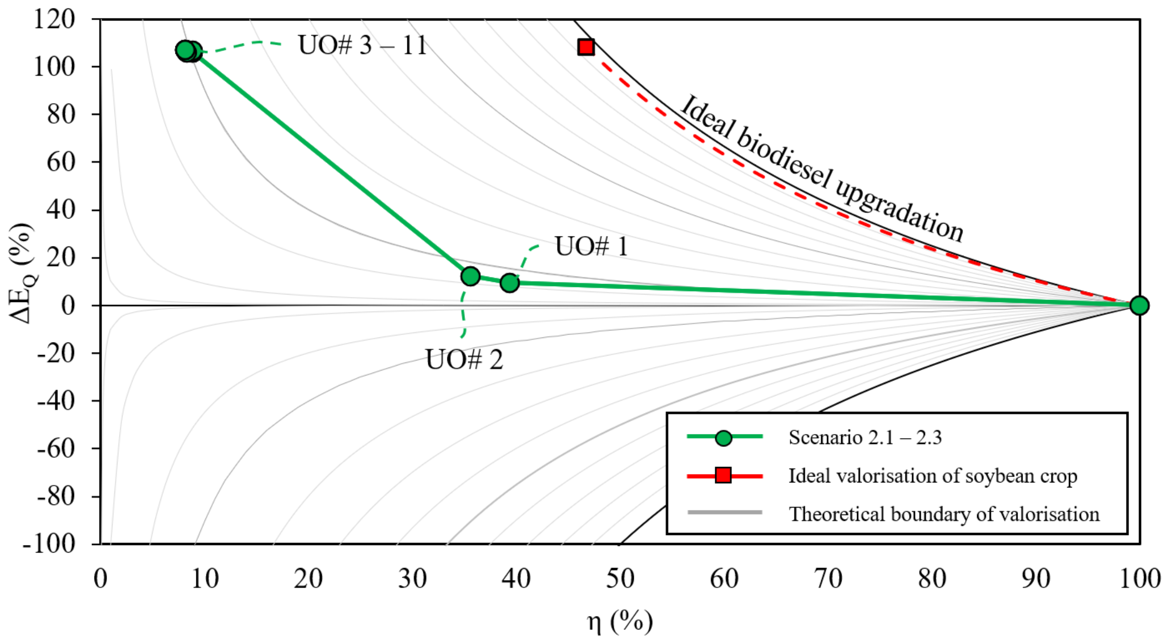

Figure 5.2: The cumulative ΔE_Q for biodiesel production. *The output of each process stage is indicated by a marker, where the unit operation number (UO#) is defined in Table 5.2.*

Table 5.2: ΔE_{Q} and η for Group 2 of biodiesel production scenarios.

No.	Unit operation	η	ΔE_{Q}
1	Harvesting	39	9
2	Bean pretreatment	36	12
3	Oil extraction	36	106
4	Oil and solvent recovery	9	106
5	Degumming	9	107
6	Hull and meal processing	9	107
7	Oil pretreatment	8	106
8	Transesterification	8	106
9	Fame purification	8	107
10	Glycerol and methanol recovery	8	107
11	Cogeneration	8	107

The immediate impression presented by Figure 5.2 is the substantial loss of mass. A final η of only 8 % is achieved: a 39 % difference between the real and the ideal case. The mass loss is predominantly attributed to the loss of soybean trash (61 % mass loss after harvesting), hulls (3 % mass loss after bean pretreatment) and the meal (27 % loss of mass after oil extraction). The crude oil is the desirable feedstock for the transesterification process. However, the isolation of the crude oil from the original biomasss yields only 9 % of the original mass. The process only encounters a further 0.6 % reduction in mass yield to obtain the final biofuel (despite the extensive operations required). It is important to note that the addition of methanol during transesterification is accounted for.

Although the soybean co-produts (hulls, meal, and glycerol) are still value added products with necessary markets, for biodiesel production, soybeans are cultivated for the recovery of crude oil. The oil makes up only a small fraction of the soybean crop which puts into question the suitability of the feedstock in the context of land-use change, resource allocation, and process efficiency.

In terms of the increase in energy density, the ΔE_{Q} progressively increases as more lignocellulose is removed: the trash, hulls, and meal have a far lower HHV than the crude oil (see Table 5.3). The increase in ΔE_{Q} is therefore only as a result of refining the biomass rather than from chemical processing. After oil extraction, ΔE_{Q} increases by 106 %. Thereafter, ΔE_{Q} only increases by a further 1 % to achieve an HHV of -40.0 MJ kg^{-1} of biodiesel. Almost no improvement in energy density is achieved after transesterification and purification. The benefit of converting the oil to FAME is the reduction of viscosity which make biodiesel suitable for use in internal combustion engines. Comparatively, the bioethanol process achieves a substantial increase in ΔE_{Q} during the fermentation stage where the desirable feedstock (saccharides) are converted to ethanol—see Section 5.3.2.

Table 5.3: Higher heating value (daf basis) for the unharvested soybean crop, the straw, meal, hulls, crude oil, and biodiesel.

	Soybean crop	Straw	Meal	Hulls	Crude Oil	Biodiesel
$\Delta_c h^{\circ}\vert_{\mathrm{HHV}}$	-19.2	-18.1	-15.3	-15.6	-39.7	-40.0

5.2.2 The cumulative ΔE_η and η for soybean to biodiesel production

The change in energy yield, ΔE_η, vs the mass yield, η, is determined on a cumulative basis to assess how much energy is transferred from the feedstock to the biofuel and in other useful-forms (electricity). The energy yield also takes into account the energy consumption that the process incurs for the biomass-to-biofuel conversion. The results of Scenario 1, 2.1, 2.2, and 2.3 are shown in Figure 5.4 and Table 5.4:

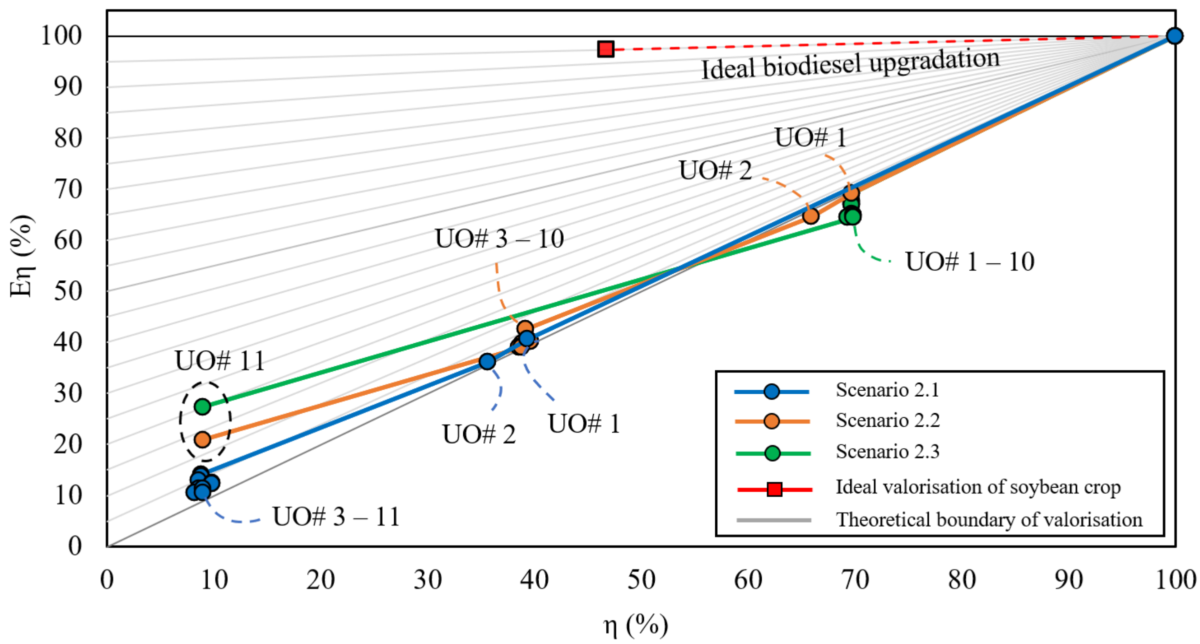

Figure 5.3: The cumulative ΔE_η for biodiesel production. *The output of each process stage is indicated by a marker, where the unit operation number (UO#) is defined in Table 5.4.*

Table 5.4: Comparison of η and ΔE_η for Group 2B of biodiesel scenarios.

No.	Unit Operation	Scenario 2.1		Scenario 2.2		Scenario 2.3	
		η	ΔE_η	η	ΔE_η	η	ΔE_η
1	Harvesting	39	41	70	69	70	69
2	Bean pretreatment	36	36	66	65	70	68
3	Oil extraction	9	14	39	43	70	67
4	Oil and solvent extraction	9	14	39	42	70	67
5	Degumming	9	13	39	42	70	67
6	Hull and meal processing	9	11	39	40	70	65
7	Oil pretreatment	8	11	39	39	69	64
8	Transesterification	10	13	40	40	70	65
9	Fame purification	10	12	40	40	70	65
10	Glycerol and methanol recovery	9	11	39	39	70	65
11	Cogeneration	9	10	9	21	9	27

After the harvesting stage, the ΔE_η is 41 % for Scenario 2.1 and 69 % for Scenario 2.2 and 2.3. When half of the trash is recovered from the field and converted to electricity, ΔE_η has increases by 70 % from Scenario 2.1 to Scenario 2.2/2.3. The recovery of straw, therefore, increases the energy recovery of the process to a large extent.

To substantiate this point, the amount of available trash needed for self-sufficiency (no fossil fuel consumption) was determined: only 17 % of the available trash is required for cogeneration to reach energy autonomy, where no hulls, meal, or glycerol is combusted.

After the oil extraction stage, the ΔE_η achieved is 14 % for Scenario 2.1, 43 % for Scenario 2.2 and 67 % for Scenario 2.3. Of course, the energy yield increases as more waste and co-products are recovered for cogeneration (trash, meal, hulls, and glycerol).

After the recovered biomass is burnt in cogeneration stage, the final ΔE_η is only 10 % for Scenario 2.1, 21 % for Scenario 2.2, and 27 % for Scenario 2.3. Evidently, for Scenario 2.2 and Scenario 2.3, there is a large reduction in ΔE_η after the recovered by- and co-products are combusted for process steam and electricity (from UO# 10–11). The observation is explained by the low energy conversion of biomass to electricity which essentially encompasses the life-cycle of biomass-to-electricity conversion.

It is quite clear that the recovery of the waste- and by-products contribute meaningfully to ΔE_η. The energy consumption of the process, however, has a minor effect. The energy consumed during the process is only 6.9 % of the energy contained in the feedstock.

Comparatively, the energy of the straw, meal, hulls, and glycerol is 83 % of the feedstock. Optimising unit operations would therefore have a marginal improvement in ΔE_η compared to improving the utilisation of waste and by-products. Even though cogeneration exhibits low conversion efficiencies (below 30 %), utilising lignocellulose for cogeneration achieves a 100 % and 161 % increase in ΔE_η for Scenario 2.2 and 2.3 compared to Scenario 2.1.

Even with the complete recovery of the by- and co-products, the final ΔE_η is far below that of the ideal case (97 %). The energy recovered from the soybean biomass in the real-life scenarios is only 10 %–27 % of the ideal ΔE_η. The composition of the soybean crop does not lend itself to efficient biodiesel recovery through transesterification.

To highlight this point, the overall η and ΔE_η were compared for two different system boundaries of Scenario 2.1:

1. The standard system boundary already evaluated (soybean crop to FAME)
2. The boundary from crude oil to FAME—crude oil is taken as the input into this process

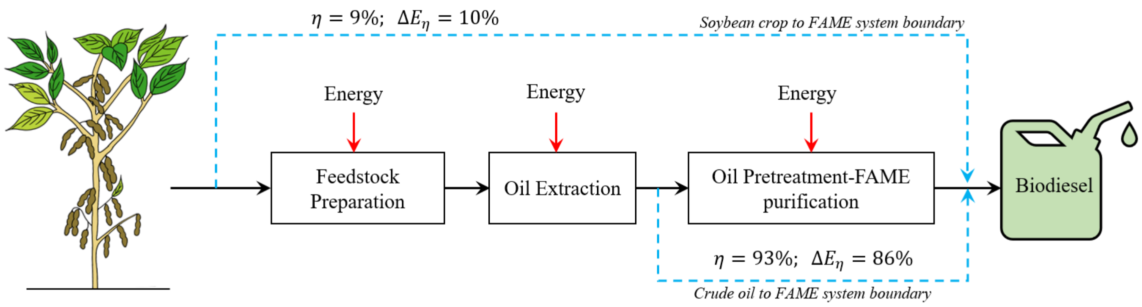

Figure 5.4: The overall η and ΔE_η for biodiesel production from the soybean crop and the crude oil. *The results are based on Scenario 2.1 where there is no recovery of the co- and by-products for cogeneration.*

When crude oil is taken as the input into the process, the results appear more favourable: η of 93 % and ΔE_η of 86 %. The comparison illustrates the energy inefficiency of utilising the soybean crop for FAME production. Using waste cooking oil for biodiesel production would yield far more favourable results than upgrading the soybean crop. Waste cooking oil does, of course, have a different chemical composition to soybean crude oil which would require further pretreatment before transesterification.

The above discussion highlights the unsuitability of the cultivated soybean crop for biodiesel production. The biomass is largely made up of lignocellulose which cannot be converted to biodiesel through industrial transesterification processes. Consequently, there is a large loss in mass that cannot be recovered in the FAME. From a sustainability perspective, the large loss in mass and energy yield essentially indicates the wasted allocation of agriculture for biofuel production which has a pronounced effect on land-use change and the food-energy nexus of the globe.

To improve the energy metrics on an industrial level, the commercialisation of alternative methods of lignocellulose upgradation is required. These methods could involve the use of oleaginous microorganisms for biodiesel production, pyrolysis of biomass by-products for the production of pyrolysis oil, or second generation processing (hydrolysis) of biomass to bioethanol.

5.3 Evaluating the configurations of bioethanol production (Group 2A and 2B)

5.3.1 Comparison of the standalone and integrated 1G and 2G processes (Group 2A)

The overall mass yield, change in energy quality, and the change in energy yield for Scenarios 2-1G, 2-2G, and 2-1G2G are shown in Figure 5.5.

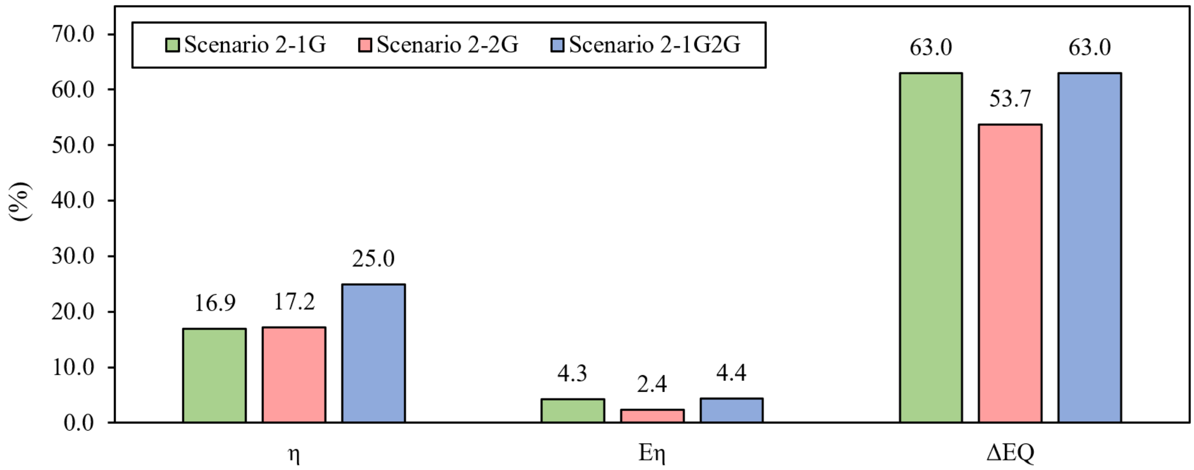

Figure 5.5: Results for Group 2A of sugarcane-bioethanol production. *The standalone 1G and 2G process, and the integrated 1G and 2G process of bioethanol production is mdoelled without the contribution of cogeneration of the by-products.*

It should be noted that for Scenario 2-1G and Scenario 2-1G2G, the input into the process is the sugarcane stalk, as with all other scenarios. However, the input into Scenario 2-2G is the lignocellulose (the sugarcane trash and bagasse only). This was chosen to evaluate the efficacy of a standalone 2G bioethanol process that valorises waste compared to a process that receives raw sugarcane. The system boundaries are illustrated in Figure 5.6:

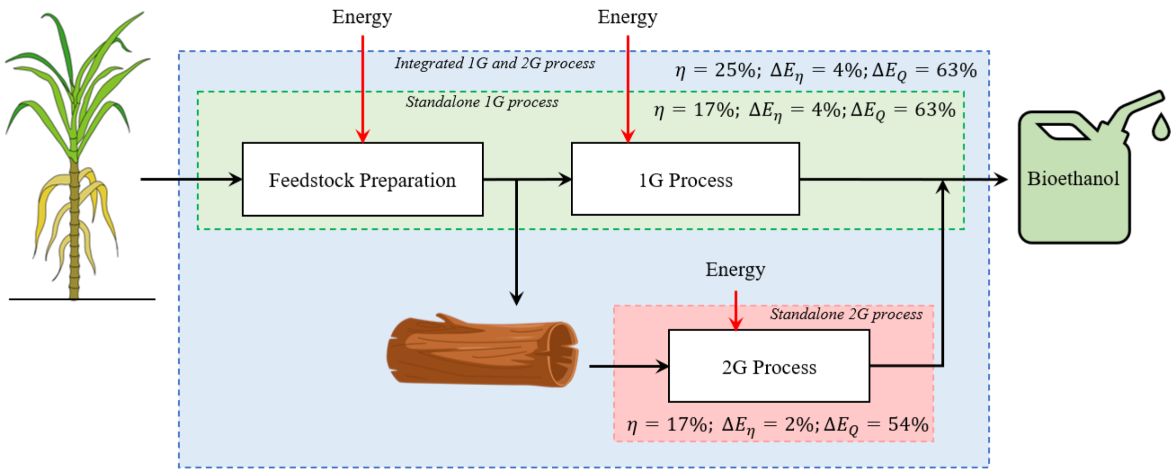

Figure 5.6: Results and illustration of system boundaries for Group 2A of bioethanol

The mass yield achieved for Scenario 2-1G and Scenario 2-2G is almost identical (≈17 %). However, the energy yield for the standalone 1G process is almost twice that of the standalone 2G process (4 % *vs.* 2 %). This result is explained by considering the input into the respective processes as well as the energy consumption.

The sugarcane into the process has a lower HHV than the lignocellulose, which is the feedstock for the 2G process (-17.8 MJ kg^{-1} *vs.* -18.8 MJ kg^{-1}). Consequently, the change in energy quality achieved for 2G production is lower than that for 1G production (54 % *vs.* 63 %). For Scenario 2-1G, the energy consumption is 20 % of the energy contained in the feedstock. For Scenario 2-2G, however, the value is 46 %. The steam explosion operation has a significantly high energy consumption for the 2G process. The higher energy consumption and lower ΔE_{Q} results the standalone 2G process achieving a lower ΔE_η than the standalone 1G process (2 % *vs.* 4 %) as less energy is recovered per unit of energy of the original feedstock.

For the integrated process (Scenario 2-1G2G), the mass yield increases by 48 % from the standalone 1G process. Of course, the trash and bagasse make up a large portion of the harvested sugarcane (63 wt. %, daf basis). When valorised for bioethanol production, a large improvement in bioethanol recovery is seen.

However, the change in energy yield exhibits a marginal increase for Scenario 2-1G *vs.* Scenario 2-1G2G (4.3 % *vs.* 4.4 %) despite the increased mass yield of bioethanol. This is due to the smaller ΔE_η achieved for the standalone 2G process, as well as high process energy consumption of the 2G process.

Considering the above, the development of 2G bioethanol production and the commercialisation thereof may be beneficial for bioethanol recovery. In terms of energy recovery, the results are less optimal where insignificant improvements are encountered in the overall process.

The above discussion is based on the process configuration where there is no cogeneration of biomass to produce process steam or electricity. Cogeneration is considered for Group 2B in the following subsection.

5.3.2 The cumulative ΔE_Q and η for sugarcane to bioethanol (Group 2B)

The change in energy quality, ΔE_Q, *vs.* mass yield, η, for sugarcane bioethanol production (Scenario 2.1–2.3) is shown in Figure 5.7 and Table 5.5.

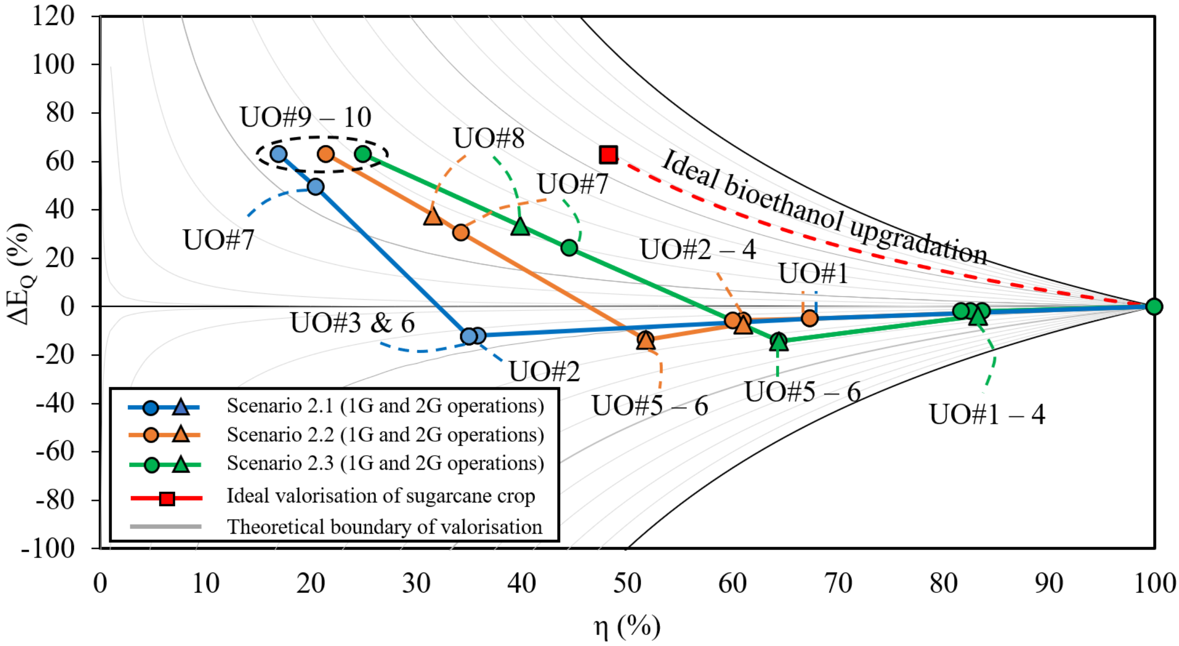

Figure 5.7: The cumulative ΔE_Q for bioethanol production—Group 2B. *The output of each process stage is indicated by a marker, where the unit operation number (UO#) is defined in Table 5.5.*

Table 5.5: Comparison of η and ΔE_{Q} for Group 2B of bioethanol scenarios.

No.	Unit Operation	Scenario 2.1		Scenario 2.2		Scenario 2.3	
		η	ΔE_{η}	η	ΔE_{η}	η	ΔE_{η}
1	Harvesting	67	-5	67	-5	84	-2
2	Milling and Cleaning	36	-12	61	-6	83	-2
3	Pretreatment	35	-13	60	-6	82	-2
4	Steam explosion (2G)	-	-	61	-7	83	-4
5	Enzymatic hydrolysis (2G)	-	-	52	-14	64	-14
6	Evap. and sterilisation	35	-13	52	-14	64	-14
7	Glucose fermentation	20	49	34	30	44	24
8	Xylose fermentation (2G)	-	-	32	38	40	34
9	Distillation and dehydration	17	63	21	63	25	63
10	Cogeneration	17	63	21	63	25	63

For the harvesting stage in Scenarios 2.1 and 2.2, there is a large drop in η (33 %) as the sugarcane trash is not valorised to the biofuel. Comparatively, there is only a drop in 16 % in mass yield for Scenario 2.3 as all of the available sugarcane trash (50 % of the total trash) is recovered for bioethanol production. The ΔE_{Q} also increases between Scenario 2.1 and 2.2 compared to Scenario 2.3 after harvesting. Sugarcane trash has a higher HHV than the stalk (-19.5 MJ kg^{-1} *vs.* -16.9 MJ kg^{-1}). When the trash is not recovered, there is a loss of energy-dense material which results in a decrease in ΔE_{Q} of the recovered material, and of course η.

The $\Delta_c h^{\circ}|_{\mathrm{HHV}}$ for the main desirable streams/components are shown below to validate the discussion:

Table 5.6: Higher heating value (daf basis) for the unharvested surgacane crop, the straw, bagasse, stalk, glucose, and bioethanol.

	Sugarcane crop	Straw	Bagasse	Stalk	Glucose	Bioethanol
$\Delta_c h^{\circ}\|_{\mathrm{HHV}}$	-17.8	-19.5	-18.4	-16.9	-14.8	-29.0

A similar result is seen for the milling stage. The sugar-rich juice is extracted after milling leaving bagasse to be recovered for bioethanol or burnt for process energy. Where more bagasse is recovered for fuel production, η and ΔE_{Q} increase.

For the 2G processing stages (steam explosion and enzymatic hydrolysis), there are only small losses in mass and a small reduction in energy quality (Scenario 2.2 and 2.3). These stages therefore exhibit marginal losses in energy dense material.

The most significant increase in ΔE_{Q} is encountered during the fermentation of glucose. There is a 269 %–495 % increase in ΔE_{Q} during this operation. Intuitively, the fermentation step is the only stage in the bioethanol process where there is a chemical upgradation of the feedstock to a product of higher HHV. The HHV of ethanol is far higher than that of glucose (-29.0 MJ kg^{-1} *vs.* -14.8 MJ kg^{-1}). However, during fermentation, there is a drop in mass yield. This is due to the fermentation reaction (Equation 3.2) where CO_2 is released; there is a reduction in the mass of bioethanol from the sugar feed. Any increase in energy density is accompanied with a decrease in mass. The same logic applies for the 2G xylose fermentation step.

We see a final increase in the change in energy quality after the purification of the sterilised wine. Here, the residual sugars and lignocellulose are separated from the ethanol, thereby increasing the final HHV.

5.3.3 The cumulative ΔE_η and η for sugarcane to bioethanol (Group 2B)

ΔE_η *vs.* η for Scenarios 2.1, 2.2, and 2.3 are shown below. As for biodiesel, the mass yield associated with ΔE_η takes into account all biomass that is recovered for biofuel production and/or process heat and electricity.

For all scenarios, the energy metrics are relatively similar for all feed preparation and pretreatment processes (UO#1–6). The similar results in the energy metrics are realised because the by-products in all scenarios are either recovered for bioethanol production or cogeneration. The recovered biomass is reflected in ΔE_η and η regardless of the end-use. Differences in the change in energy yield and mass yield will only arise due to the inefficiencies associated with the biofuel conversion process or combustion process.

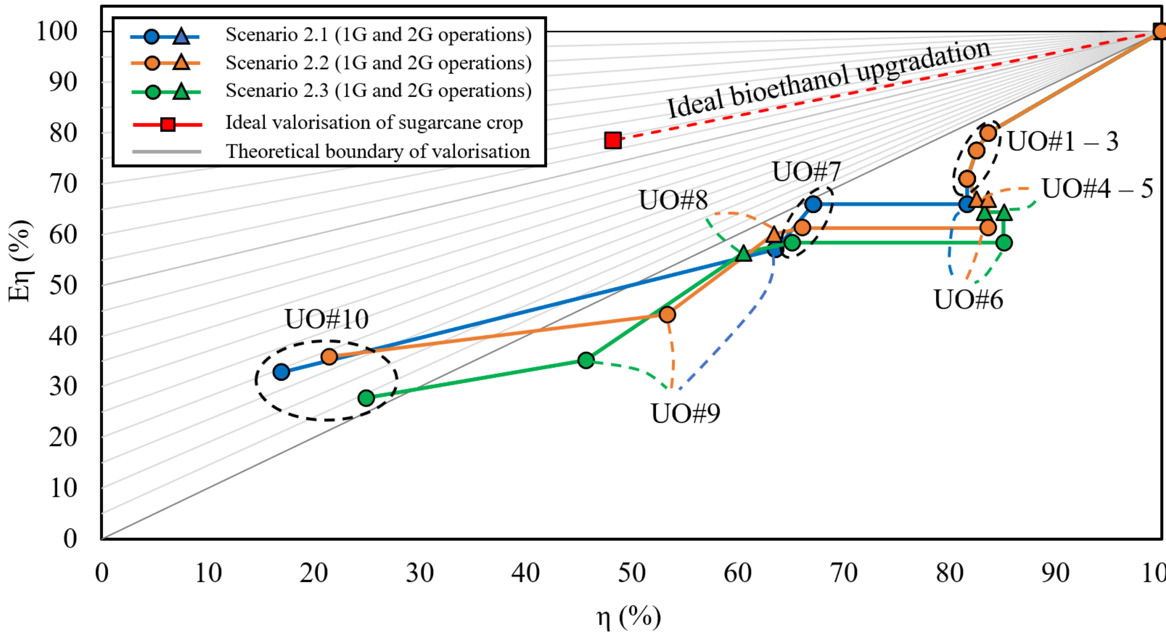

Figure 5.8: The cumulative ΔE_η for bioethanol production—Group 2B. *The output of each process stage is indicated by a marker, where the unit operation number (UO#) is defined in Table 5.7.*

Table 5.7: Comparison of η and ΔE_η for Group 2B of bioethanol scenarios.

No.	Unit Operation	Scenario 2.1		Scenario 2.2		Scenario 2.3	
		η	ΔE_η	η	ΔE_η	η	ΔE_η
1	Harvesting	84	80	84	80	84	80
2	Milling and Cleaning	83	77	83	77	83	77
3	Pretreatment	82	71	82	71	82	71
4	Steam explosion (2G)	-	-	83	67	83	64
5	Enzymatic hydrolysis (2G)	-	-	84	67	85	64
6	Evap. and sterilisation	82	66	84	61	85	58
7	Glucose fermentation	67	66	66	61	65	58
8	Xylose fermentation (2G)	-	-	63	60	61	56
9	Distillation and dehydration	64	57	53	44	46	35
10	Cogeneration	17	33	21	36	25	28

There is a slight decrease in the energy yield from for Scenario 2.2 and 2.3 during the 2G pretreatment and hydrolysis steps. The behaviour is due to the associated losses for these operations as well as the high energy consumption for steam explosion (-2683 MJ per tonne lignocellulose processed). The decrease in ΔE_η after evaporation and sterilisation is due to the energy consumption entirely (-337 MJ per tonne sugarcane processed).

After the distillation and dehydration of the ethanol, the mass yield and energy yield is highest for Scenario 2.1 (64 % and 57 % respectively) because all the available lignocellulose has been recovered for cogeneration. Comparatively, a portion of the biomass by-products in Scenario 2.2 and 2.3 have undergone conversion to bioethanol where the process inefficiencies have already been reflected in η and ΔE_η.

After the combustion of the available biomass, the overall results may be compared. The mass yield is expectedly the lowest for Scenario 2.1 (17 %), followed by Scenario 2.2 (21 %) and Scenario 2.3 (25 %). After conversion of lignocellulose to process energy, the only mass remaining is that of the biofuel. Therefore, the mass yield is highest for Scenario 2.3, where bioethanol production is maximised. The maximum in η does not necessarily indicate where ΔE_η will be the highest. The overall optimum of ΔE_η is obtained for Scenario 2.2 (36 %) where the bioethanol production plant is exactly at the point of energy autonomy and where all the excess lignocellulose is used for bioethanol production. In comparison, the ΔE_η for Scenario 2.3 is 28 % and for Scenario 2.1, it is 33 %. Even by maximising the energy recovery through integrating second generation processing (Scenario 2.2), the ΔE_η achieved is only 3 % higher than traditional first generation bioethanol production (Scenario 2.1). There is a marginal increase in energy yield by integrating the 2G process. A techno-economic study would be required to justify the additional infrastructure associated with the 2G production process.

Evidently, converting all available biomass by-products to process heat and electricity (Scenario 2.1) has a more favourable energy recovery than maximising bioethanol production (Scenario 2.3). This sentiment is expanded on in Section 5.3.4, where the sensitivity analysis is evaluated.

The energy consumption for the overall process is about 20 % (Scenario 2.1), 26 % (Scenario 2.2) and 30 % (Scenario 2.3) of the feedstock energy. However, the energy contained in the straw and bagasse is 67 % of the feedstock energy. The energy potential of the lignocellulose has a more significant effect on ΔE_η than just the energy utility of the process operations. In essence, there is a trade-off between utilising waste biomass for bioethanol production and for process energy.

Compared to the ideal route of upgradation, the overall η achieved for all scenarios is only 8 %–12 % of the ideal; and the overall ΔE_η achieved for all scenarios is only 22 %–29 % of the ideal. The energy utility, combined with the process inefficiencies result in poor energy metrics compared to the ideal case.

5.3.4 The point of energy self-sufficiency

Scenario 2.2 for bioethanol production is based on the point where energy self-sufficiency is reached for the processing facility. At this point, the boiler is no longer supplemented by fossil fuels to produce steam and electricity for the plant.

A sensitivity analysis was performed to iteratively solve for this point. First, all the trash is burnt in the boiler and the amount of bagasse sent to cogeneration was increased. All of the trash was combusted first in this model because the trash alone does not release enough energy to completely replace the fossil fuel requirements of the boiler. Therefore, the boiler must be supplemented by all the available trash and some bagasse. The trash was chosen as the first lignocellulose to be combusted as traditional bioethanol plants incinerate the trash for waste disposal regardless.

It was determined that 17 % of the available bagasse (and all of the available trash) must be combusted to obtain a self-sufficient plant. At this point, 83 % of the bagasse is available for 2G bioethanol production.

It is important to note that at the point of energy self-sufficiency, a maximum in the ΔE_η is achieved (36 %), as shown in Figure 5.9. This behaviour is intuitive when taking into account the conversion efficiency achieved for each section of the Figure.

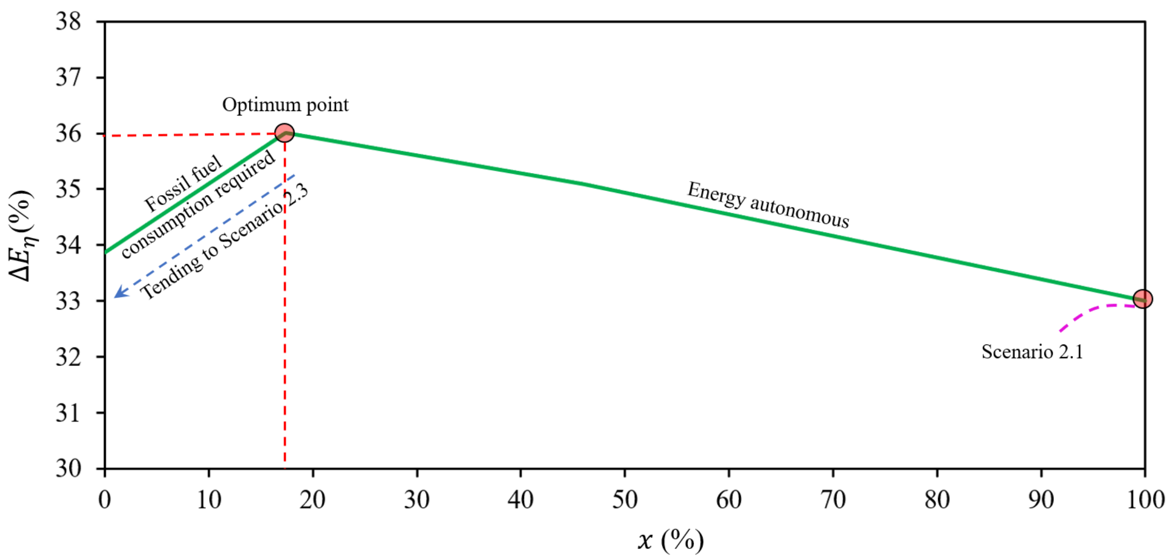

Figure 5.9: The sensitivity analysis performed to determine the amount of bagasse diverted to cogeneration (x) for the optimisation of ΔE_η. *All of the available sugarcane trash is sent to cogeneration for this analysis.*

Before the optimum point, fossil fuels are used to supplement the boiler which reduces the energy yield. As fossil fuels are increasingly replaced with biomass, the energy yield increases. Of course, as more bagasse is diverted away from the 2G process, the steam demand for the 2G process also decreases and the bioethanol production decreases. This indicates that the consumption of fossil fuels and the conversion in the boiler thereof overwhelms the benefit of energy production from the bioethanol yield.

However, after the point of reaching self-sufficiency (optimum point), the energy yield starts to decrease. This behaviour indicates that after the optimum point, the energy produced in the form of electricity is less than the energy yielded from biofuel valorisation, even though the power demand of the 2G process increases along the x-axis.

It is also interesting to note the slopes of the left hand and right hand side of the optimum point. Below the value of $x = 17$ %, ΔE_η tends towards the overall results of Scenario 2.3 at a faster rate (per unit x) than on the right hand side of the optimum point. It is therefore more desirable to have a higher production of excess electricity from process waste biomass than to maximise bioethanol production.

5.4 Cross-process comparison and end-point utilisation

This section aims to evaluate 1) the sugarcane-bioethanol process *vs.* soybean-biodiesel process and 2) the end-use of the biofuels in an internal combustion engine *vs.* the conversion of the feedstock directly to electricity.

5.4.1 Sugarcane to bioethanol *vs.* soybean to biodiesel

To compare the two biofuel production processes, scenarios with similar conditions are considered. Firstly, Scenario 2-1G (for bioethanol) and Scenario 2.1 (for biodiesel) are compared as these are process scenarios with similar conditions. Both scenarios consider 1G production where there is no cogeneration of the biomass co- and by-products. For the overall processes, the bioethanol process achieves almost double the mass yield compared to biodiesel production (17 % *vs.* 9 %). However, the change in energy yield is far less (4 % *vs.* 10 %). The higher ΔE_η for soybean valorisation is attributed mainly to the larger ΔE_Q achieved (107 % for soybean-biodiesel and 63 % for sugarcane-bioethanol) and the lower energy consumption per energy unit of the feedstock (7 % for soybean-biodiesel and 20 % for sugarcane-bioethanol).

The results for ΔE_η change considerably when introducing the complete cogeneration of the biomass co- and by-products (Scenario 2.1 for bioethanol and Scenario 2.3 for biodiesel). ΔE_η increases by 725 % for sugarcane processing and 170 % for soybean processing. Cogeneration of the by-products improve the energy metrics of bioethanol far more than that of biodiesel. To explain the difference, the energy profile of the feedstocks should be considered:

Table 5.8: Energy profile of the soybean and sugarcane crops (unharvested, daf).

Component	Soybean crop MJ MJ^{-1}	Sugarcane crop MJ MJ^{-1}
Straw/trash	57 %	36 %
Processing by- and co-products	24 %	32 %
Biofuel-specific feedstock	19 %	32 %

Straw/trash: the total before harvesting

Processing by- and co-products: the bagasse or meal/hulls recovered after feedstock preparation

Biofuel-specific feedstock: saccharides for bioethanol and oil for biodiesel

The soybean trash constitutes 57 % of the cultivated crop. Whereas for sugarcane, the trash is only 36 %. Both models consider leaving 50 wt. % of the trash on the field for soil fertilisation. The abandonment of half of the straw results in a significant reduction in energy yield. The effect is felt far less for sugarcane to bioethanol production as the straw constitutes less of the crop's total energy.

Through the above discussion as well as the results presented in the previous subsections, it becomes increasingly evident that the composition of the biomass into the process must be considered when evaluating the overall energy efficiency of the process. The energy recovery of biofuel production is far more dependent on the suitability of the feedstock than the utility requirements of the individual unit operations. Sugarcane-bioethanol production is less affected by the feedstock composition because the biomass by-products may undergo the 2G process for bioethanol production. However, soybean lignocellulose by-products cannot undergo industrial transesterification for biodiesel production—the biomass may only be considered for cogeneration. The latter aspect may be improved by considering an integrated biodiesel-bioethanol production plant, or by considering other methods of upgrading the soybean lignocellulose. This, however, is beyond the scope of this study.

5.4.2 The end use of biofuels

Scenario 3 represents the end use of the liquid biofuel in an internal combustion engine which is based on the biofuel production of Scenario 2.2 for both the bioethanol and biodiesel process. Scenario 4, on the other hand, encompasses the direct conversion of the harvested biomass to electricity. The mass yield and change in energy quality is 0 % and -100 %, respectively, for both Scenarios—there is no mass of energy dense material retained after the whole life cycle. Conversely, the energy yield is greater than 0 % as energy is still produced either in the form of mechanical or electrical energy. For Scenario 3, the energy yield is always less than Scenario 2 because conversion inefficiencies are introduced for the end-use of the fuel.

For Scenario 3, the combustion of bioethanol and biodiesel to mechanical energy results in a drop in ΔE_η by 17 % and 19 % respectively. Comparatively, combusting the biomass crop for electricity generation achieves a 3 %–8 % higher energy yield than the crop-to-fuel-to-wheel process. Converting the biomass directly to electricity has a significant increase in energy efficiency in comparison to undergoing biomass valorisation for use in an engine. Of course, this is an abortive comparison as liquid biofuels are a necessary energy storage system for transportation utility. Regardless, this comparison illustrates the magnitude of wasted energy inherent in biomass to biofuel production processes.

Table 5.9: Bioethanol and biodiesel model results.

Scenario	Biofuel produced[1] (kg ton^{-1}_{bm})	Electricity surplus[1] (kWh ton^{-1}_{bm})	Steam utility[1,3] (kg ton^{-1}_{bm})	Excess steam [1,4] (kg ton^{-1}_{bm})	η^2 (%)	$\Delta E_Q{}^2$ (%)	$\Delta E_\eta{}^2$ (%)	Net energy produced[1,5] (MJ ton^{-1}_{bm})
Sugarcane bioethanol								
1	185	-	-	-	48	63	79	5357
2-1G	65	36	458	0	17	63	4	291
2.1	65	139	458	346	17	63	33	2244
2.2	82	58	633	0	21	63	36	2456
2.3	96	71	749	0	25	63	28	1896
3	-	58	633	0	0	-100	9	665
4	-	976	0	949	0	-100	12	837
Soybean biodiesel								
1	1099	-	-	-	47	107	97	43971
2.1	164	0	486	0	9	107	10	4116
2.2	164	654	486	2250	9	107	21	8191
2.3	164	1363	486	4649	9	107	27	10743
3	-	654	486	2250	0	-100	8	3268
4	-	6863	-	6680	0	-100	16	5953

ton_{bm}: Ton of biomass processed (*i.e.* soybeans and sugarcane stalk sent to processing plant respectively)

[1] As received basis | [2] Dry and ash free basis

[3] Steam consumed by biofuel production process | [4] Steam expanded in condensing steam turbine for surplus electricity

[5] Net energy: Total energy produced in the form of biofuel/electricity/steam minus the fossil fuel derived energy consumed

5.5 Closing the gap of conventional energy metrics

The fossil energy ratio (FER), the net energy ratio (NER), and the change in energy yield (ΔE_η) are compared for Scenarios 2.1, 2.1, 2.3, 3 and 4 for the soybean biodiesel model (Figure 5.10). The below discussion is applicable to the sugarcane-bioethanol process scenarios as well. Only the soybean-biodiesel results are discussed for simplicity.

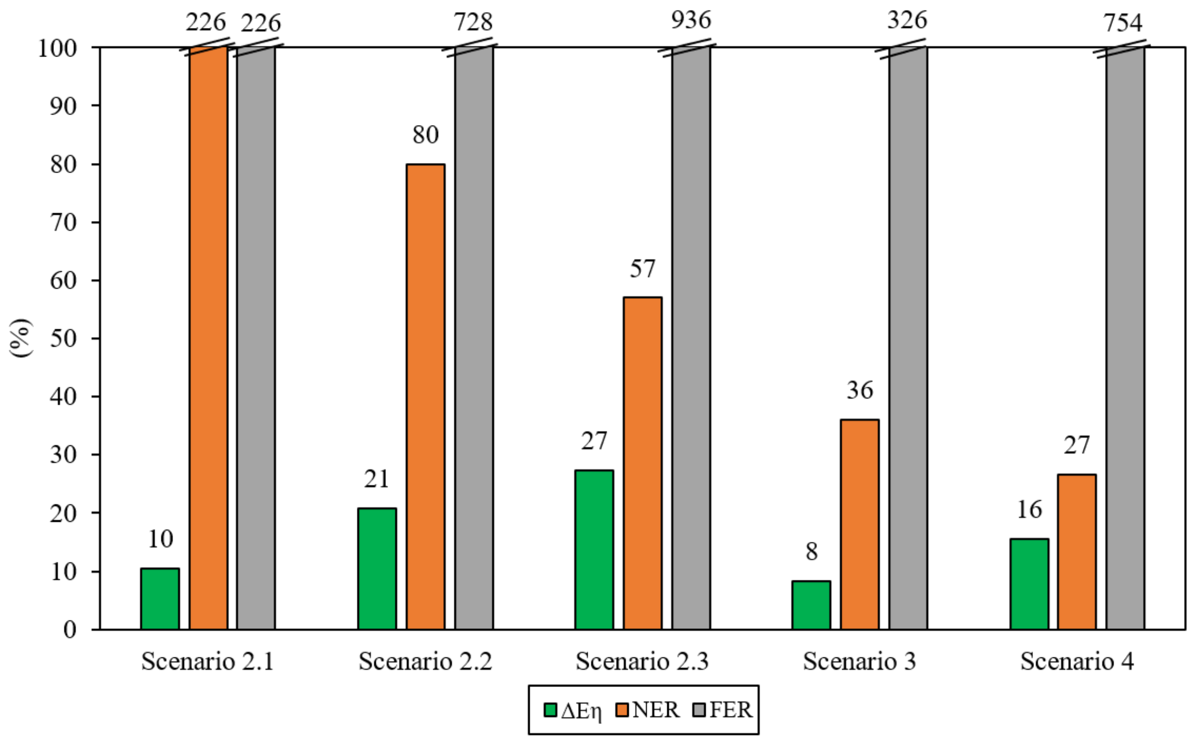

Figure 5.10: The overall values for ΔE_η, NER and FER for the biodiesel model scenarios. *The y-axis is limited to 100 % as some values exceed this limit to such as extent that the comparison would otherwise be diluted.*

The main difference between the definition of life-cycle assessment metrics (FER and NER) and the energy metrics of this study is the reference state of energy consumption. ΔE_η considers the biomass feedstock, in its entirety, as the main energy input. The change in energy yield increases based on the net energy production in reference to the biomass cultivated. In contrast, the NER only considers biomass as an input if it is recovered for conversion to process heat or electricity—the NER does not take into account the biomass utilised for biofuel production. The FER does not consider biomass as an energy cost at all, and only looks at the total energy produced in reference to the fossil fuel consumed.

The FER increases as fossil fuels are increasingly replaced by biomass for the production of process steam and electricity. The FER increases from 226 % (Scenario 2.1), to 728 % (Scenario 2.2) and to 936 % (Scenario 2.3). This parameter communicates that the biodiesel production process produces 2.26–9.36 times more energy than what is consumed in non-renewable fuels. The FER conveys whether the process may overcome non-renewable fuel consumption. This is a fair enough indication of the fossil fuel demand of the process. However, the FER does not convey how efficiently energy is utilised or transferred from the feedstock to the product.

The NER paints a different picture. For Scenario 2.1, the NER is equal to the FER (226 %) as no biomass is consumed for thermal/electrical process energy. As more biomass is diverted to cogeneration, the NER drastically decreases and begins to approach results of the ΔE_η but in an inverse relationship. The NER initially indicates that Scenario 2.1 produces 2.26 times more energy than what is consumed, but reduces to value of 0.57 (Scenario 2.3). The NER is initially high for Scenario 2.1 because the reference of energy consumption is only the fossil fuel. The NER only considers biomass as energy input when biomass is converted to process energy in cogeneration (Scenario 2.2 and Scenario 2.3).

The message of the NER results are counter-intuitive. The NER is meant to give a measure of renewability. However, as our biodiesel production plant becomes more energetically self-sufficient (Scenario 2.1 *vs.* Scenario 2.3), the "renewability factor" dwindles. This illustrates the inherent flaw of excluding the biomass feedstock as a direct energy input at the initial stage of the system boundary.

In contrast, the energy yield, ΔE_η, increases as more biomass waste/co-products are diverted to generate thermal/electrical process energy. When waste/co-product streams that are not valorised are utilised for useful energy (biofuel or electricity), the gain on energy investment is greater.

Lastly, the NER indicates that Scenario 3 is less renewable than Scenario 4 (NER value of 36 % and 27 % respectively). Scenario 3 has far more inefficiencies as it involves valorising the soybean crop to biodiesel and then converting it to mechanical energy. The TTW stage alone has an efficiency of 25 % (where only 25 % of the biodiesel energy is recovered in mechanical energy). Comparatively, the energy conversion of combusting the feedstock directly to electricity is 18 %. There is a small amount of fossil energy consumed in Scenario 4 due to the cultivation and harvesting energy requirements. Again, the NER values provide a false indication of which scenario provides a higher recovery of energy. In contrast, the change in energy yield conveys results which are inline with the process efficiencies (ΔE_η of 8 % and 16 % for Scenario 3 and Scenario 4 respectively).

Of course, the results for NER and FER are not directly comparable with results obtained in life-cycle assessments: the system boundary of this study is different to that of life-cycle assessments; the developed models do not consider the life-cycle energy equivalent of material and energy inputs; and mass or energy allocation methods are not applied.

Regardless, this comparison does serve to identify a gap in the reliability and sensibility of the FER and NER that ΔE_η addresses.

5.6 Food-crop for thought

It would be naive to suggest that all processing operations, biomass- or petroleum-derived, have been developed and adopted because of favourable energy metrics. Dale (2007) presents a compelling argument dispelling the use of energy metrics to evaluate biofuel processes—specifically for the net energy ratio. The author highlights that energy products are refined based on the service they provide, rather than the process efficiency. This is the very reason why global markets value electricity and liquid fuels far more than coal or crude oil; it is the quality of the energy carrier rather than the calorific value that determines the demand.

Even so, analysing ΔE_η provides invaluable insight into the suitability of the feedstock and efficiency of the process. The energy recovered from the feedstock must be understood in the context of the biofuel industry. With the every growing demand for bioethanol and biodiesel, it is energetically inefficient to divert food supplies and agricultural land to biofuels, where small ΔE_η are achieved. This is especially concerning when biomass-derived fuels are considered as a viable substitute for non-renewable fuels. Fossil fuels are demonised for their environmental impact. However, the feedstocks from which they are derived are appropriate for their synthesis (*e.g.*, crude oil and natural gas). Thus, even in the environmental and sociological context, ΔE_η is an imperative starting point to assess the efficacy of fuel synthesis.

Chapter 6: Conclusions and recommendations

This dissertation presents a criticism of industrially employed biofuel production processes and traditional energy metrics. The change in energy quality and the change in energy yield were assessed for the soybean-biodiesel and the sugarcane-bioethanol production processes for various scenarios. The scenarios explored encompass the use of the waste- and by-products for process energy and biofuel production, as well as the end-use of the biofuel and the direct conversion of the biomass crop to electricity.

The ΔE_{Q} achievable for soybean-biodiesel production is 107 %. Almost the entire increase in ΔE_{Q} is attributed to extracting the crude oil. The transesterification step does not serve to improve the quality of the fuel, but to produce a fuel with suitable physical characteristics for engines. Even with the large increase in energy density, there is a relatively small recovery of energy in the product relative to the feedstock. ΔE_{η} for the the biodiesel process is 10 %–27 %, where the change in energy yield increases significantly as more of the waste- and by-products are used in cogeneration. Even with the utilisation of all available by-product streams, ΔE_{η} is only 28 % of the ideal case. The poor recovery of energy materialises because the soybean crop is only composed of 19 % oil (MJ MJ^{-1}), where the balance is made up of the straw, meal, and hulls.

For the sugarcane-bioethanol process, the ΔE_{Q} is 63 %. It was shown that for an integrated 1G and 2G bioethanol process, ΔE_{η} favours the production of process energy from lignocellulose rather than the 2G production of bioethanol. There is an optimum value of ΔE_{η} (36 %) which is achieved where just enough lignocellulose is used for process energy and the balance for bioethanol production. Even so, the ΔE_{η} in this case is only 3 % higher than the traditional 1G process where all the lignocellulose is combusted for process energy. Despite the good intentions of maximising bioethanol yield from waste lignocellulose in 2G production, the energy losses indicate that 2G production is simply not worth the energy, especially considering the additional infrastructure required. In terms of the ideal case, Group 2B of the scenarios achieved 35 %–46 % of the ideal ΔE_{η}, where the ΔE_{η} for for bioethanol production is far more favourable than the biodiesel process. This is predominantly attributed to the fact that the sugarcane feedstock is composed of less straw.

It was shown that the life-cycle of the feedstock-to-fuel-to-mechanical energy in an internal combustion engine results in more energy losses than converting the biomass feedstock directly to electrical energy. This theoretical exercise depicts the process inefficiencies encountered in production processes.

Regardless of the modelled scenario, food-based crops are not viable feedstocks for fuel upgradation. Even for bioethanol production, upgrading lignocellulose to bioethanol does not provide favourable energy metrics. In comparison, the conversion of crude oil to biodiesel holds a significant improvement. Therefore, the importance of considering the feedstock used for biofuel production cannot be understated.

Finally, the net energy ratio (NER) and the fossil energy ratio (FER) were compared to the ΔE_η for soybean-biodiesel production of Group 2, 3, and 4 of the model scenarios. The NER and FER are shown to be poor metrics for evaluating the energy efficiency of biofuel processes. Although the FER provides an intuitive measure of the renewability of the process regarding fossil fuel consumption, the results become meaningless when biomass is used for process energy. The NER produces results which are counter-intuitive to the essence of a "sustainable" processes—as more biomass is used for cogeneration, the NER decreases. This flaw is inherent to the definition of the NER. It highlights the importance of considering the entire biomass plant as the reference state for an energy-metric-based evaluation.

This study may be extended into various fields of research concerning biomass valorisation. The following is recommended:

1. The integrated bioethanol and biodiesel process may be evaluated based on the change in energy yield and change in energy quality. The sugarcane straw as well as the soybean straw and co-products (meal and hulls) may be used to produce 2G bioethanol. An optimal configuration of these integrated plants may be subsequently determined.
2. The energy metrics may be applied to biofuel production processes for different feedstocks—the suitability of the feedstock, specifically, should be evaluated.
3. This study should be extended into several more biomass valorisation processes (that are not yet commercialised). These include pyrolysis, hydrothermal liquefaction, gasification, and others.
4. The change in energy quality and the change in energy yield should be evaluated in terms of life-cycle assessment system boundaries and parameters. In this regard, the energy metrics may serve to enrich life-cycle assessment studies that intend to quantify energy utilisation and the sustainability of biofuel production.
5. This study has exhibited the inefficiencies encountered in biomass-derived fuel production. Care should be taken when framing biofuels as a promising substitute for non-renewable fuels. Subsequently, the naturally guided biomass-to-fuel synthesis pathways should be assessed against traditional fossil fuel production.

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Appendix A: Biodiesel model parameters

All parameters for the biodiesel model are taken from Sheehan *et al* (1998) unless otherwise indicated.

A.1 Mass balance parameters

Table A.1.1: Process parameters for cultivation and harvesting, and soybean oil and meal preparation.

Parameter	Value	Unit
Cultivation & Harvesting		
Straw yield [a]	1.35	kg kg_{beans}^{-1}
Straw left on the field [b]	50	wt. %
Cleaning & drying		
Final moisture in beans	10.50	wt. %
Dehuller		
Meal lost	0.65	wt. %
Oil lost	0.58	wt. %
Hulls recovered	99.00	wt. %
Moisture with hulls	0.74	wt. %
Conditioner		
Final bean moisture	9.00	wt. %

[a] Martelli-Tosi *et al* (2017), Bose & Martins Filho (1984), and Lopes *et al* (2020)

[b] De Pretto, Tardioli & Costa (2017)

Table A.1.2: Process parameters for cultivation and harvesting, and soybean oil and meal preparation (continued).

Parameter	Value	Unit
Oil extraction		
Total hexane used	1.2	kg $kg_{flaked\ beans}^{-1}$
Make-up hexane	0.0024	kg $kg_{flaked\ beans}^{-1}$
Recovered hexane	1.1976	kg $kg_{flaked\ beans}^{-1}$
Oil concentration in miscella	23.50	wt. %
Oil recovered in miscella	96.00	wt. %
Hexane concetration with the flakes	35.00	wt. %
Oil recovery		
Hexane recovery	100.00	wt. %
Oil lost	0.00	wt. %
Solvent recovery		
Hexane recovery	99.80	wt. %
Hull and meal processing		
Meal moisture after toaster	18.00	wt. %
Meal moisture after drying	14.00	wt. %
Meal moisture after cooler	12.00	wt. %
Final hull moisture *	19.00	wt. %

* Assumed based on mass balance by Granjo, Duarte & Oliveira, 2017

Table A.1.3: Process parameters for degumming and alkali refining.

Parameter	Value	Unit
Degumming		
Total oil loss	3.11	wt. %
Oil lost from triglyceride [a]	0.476	wt. %
Oil lost from phosphatides [a]	2.50	wt. %
Oil lost from unsaponifiable matter [a]	0.134	wt. %
Water addition	75	wt. % of phosphatide mass
Water content in gum/oil mixture [b]	5.00	wt. %
Alkali refining		
NaOH stoicheometric excess	113	%
Wash water addition	15	wt. % of oil
Oil lost from FFAs	0.719	wt. %
Oil lost from Triglycerides	1.799	wt. %
Oil lost from Unsaponifiable matter	1.485	wt. %

[a] Calculated

[b] Assumed

Table A.1.4: Process parameters for soybean oil conversion.

Parameter	Value	Unit
Transesterification		
Methanol:oil ratio	6:1	mol mol^{-1}
NaOH [a]	1.0	wt. % of oil
2 Reactant temperature	60	°C
Overall triglyceride conversion	99	wt. %
Aqueous phase carried over to FAME	5.0	wt. %
FAME purification (Overall)		
Ester phase recovered	100	wt. %
Moisture in ester product	0.00	wt. %
Overall aqueous phase recovery	100	wt. %
Glycerol and methanol recovery		
Fist distillation: Glycerol bottoms water content	20	wt. %
Second distillation: methanol in bottoms	0.5	wt. %
Second distillation: water in distillate	0.5	wt. %
Overall glycerol recovery	100	wt. %
Overall methanol recovery	99	wt. %

[a] Myint & El-Halwagi (2009)

A.2 Energy consumption parameters

Table A.2.5: Energy inputs for harvesting and cultivation. *Average of Castanheira* et al *(2015), Pimentel & Patzek (2005), Pradhan, Shrestha, McAloon, Yee, Haas & Duffield (2011), and Sheehan* et al *(1998).*

Utility	Value MJ t_{beans}^{-1}
Diesel	622
Petroleum	253
LPG	21.1
Natural gas	14.3
Electricity	12.7

Table A.2.6: Energy inputs for soybean oil extraction and meal and hull processing.

Component	Electricity MJ t_{beans}^{-1}	Steam MJ t_{beans}^{-1}	Natural gas MJ t_{water}^{-1}	Hexane MJ $t_{flaked\ beans}^{-1}$
Soybean preparation				
Cleaning	-14.33			
Drying	-55.8		-3.489 [a]	
Cracking	-14.90			
Dehulling	-8.50			
Conditioning	-4.07	-173.35		
Flaking	-50.26			
Hexane extraction				
Oil extraction	-12.96			-117.67

[a] Erickson, 2015

Table A.2.7: Energy inputs for soybean oil extraction and meal and hull processing (continued).

Component	Electricity MJ t_{beans}^{-1}	Steam MJ t_{beans}^{-1}	Natural gas MJ t_{water}^{-1}	Hexane MJ $t_{flaked\ beans}^{-1}$
Hull and meal processing				
Desolventizer toaster	-14.90	-421.85		
Meal dryer	-2.304	-85.96		
Meal cooler	-9.144			
Meal grinding	-26.064			
Hull grinding	-19.44			
Hull toaster		-48.97		
Oil recovery				
First effect evaporator	-0.54			
Second effect evaporator	-0.54	-41.748		
Third effect evaporator	-0.288	-45.338		
Solvent recovery				
Solvent recovery	-1.872			
Waste treatment	-1.872	-36.811		
Degumming				
Hydration	-0.864	-36.811		
Centrifuge	-2.448			
Dryer	-2.772	-32.397		

Table A.2.8: Energy inputs for degumming and alkali refining.

Component	Electricity MJ t_{beans}^{-1}	Steam MJ t_{beans}^{-1} or MJ $t_{biodiesel}^{-1}$
Degumming		
Hydration	-0.864	-36.028 MJ t_{beans}^{-1}
Centrifuge	-2.448	
Drying	-2.772	-32.397 MJ t_{beans}^{-1}
Alkali refining		
Crude oil heater		-108.515 MJ $t_{biodiesel}^{-1}$
Wash water heater		-32.554 MJ $t_{biodiesel}^{-1}$
Preheater for vacuum dryer		-9.784 MJ $t_{biodiesel}^{-1}$
Vacuum dryer		-4.013 MJ $t_{biodiesel}^{-1}$

Table A.2.9: Energy inputs for oil conversion.

Component	Electricity MJ t_{beans}^{-1}	Steam MJ $t_{biodiesel}^{-1}$
Transesterification		
First reactor		-97.012
Second reactor		-10.119
FAME purification		
Wash water heater		-41.914
Ester heater		-104.786
Preheater for vacuum dryer		-83.848
Vacuum dryer		-2.285
Glycerol recovery		
Glycerine preheater		-75.591
Distillation reboiler		-57.264
Methanol recovery		
Methanol dryer		-224.580

Appendix B: Bioethanol model parameters

B.1 Mass and energy balance parameters

Table B.1.1: Process parameters for cultivation and harvesting, and 1G bioethanol production.

Parameter	Value	Unit
Cultivation and Harvesting		
Fossil fuel energy consumption	-139	MJ t_{cane}^{-1}
Sugarcane straw produced (dry) [c]	140	kg t_{cane}^{-1}
Straw moisture [c, g]	15	wt. %
Straw recovered from the field [a]	50	wt. %
Cleaning		
Dirt removed	90	wt. %
Milling		
Bagasse yield (wet)	240	kg t_{cane}^{-1}
Bagasse moisture content [a, b]	50	wt. %
Sugar recovery [i]	97	wt. %
Water for imbibition [e]	0.28	t t_{cane}^{-1}
Electricity consumption	16 [f]	kWh t_{cane}^{-1}
Pre-treatment		
Preheating steam consumption (2.5 bar) [d]	70.25	kg t_{cane}^{-1}
CaO concentration [a]	10	wt. %
CaO flowrate [a]	2	kg t_{juice}^{-1}
Steam consumption (2.5 bar) after liming [d]	68.49	kg t_{cane}^{-1}
Sugar recovery after juice treatment [c]	99.5	wt. %
Clarified juice sugar concentration [f]	15	wt. %

Table B.1.2: Process parameters for cultivation and harvesting, and 1G bioethanol production (continued).

Parameter	Value	Unit
Evaporation and sterilisation		
Steam consumption (2.5 bar) for evaporation [d]	114.14	kg t_{cane}^{-1}
Sucrose concentration after evaporation [f]	22	wt. %
Steam consumption (2.5 bar) for sterilisation [d]	32.14	kg t_{cane}^{-1}
Fermentation		
Sucrose to glucose mass yield [*]	100	wt. %
Glucose to ethanol mass yield [f]	90.48	wt. %
Distillation and dehydration		
Hydrous ethanol concentration [e]	93	wt. %
Steam consumption (2.5 bar) for azeotropic distillation [c]	1.5	kg L^{-1}_{EtOH}
Anhydrous ethanol concentration [e]	99.6	wt. %
Steam consumption (2.5 bar) for dehydration [h]	0.6	kg L^{-1}_{EtOH}
Overall ethanol recovery [c]	99.7	wt. %
Density of bioethanol [j]	789	kg m^{-3}
Auxiliary operations		
Electricity consumption [c]	-30	kWh t_{cane}^{-1}

[*] Assumed

[a] Furlan, Tonon Filho, *et al* (2013)

[b] Carvalho *et al* (2020)

[c] Dias, Cunha, Jesus, Rocha, *et al* (2011)

[d] Dias, Modesto, *et al* (2011)

[e] Dias, Junqueira, Cavalett, Pavanello, *et al* (2013)

[f] Dias, Ensinas, *et al* (2009)

[g] Oliveira, Pinheiro, *et al* (2013)

[h] Dias, Junqueira, Cavalett, Cunha, Jesus, Rossell, *et al* (2012)

[i] Modesto, Zemp & Nebra (2009)

[j] Muhaji & Sutjahjo (2018)

Table B.1.3: Process parameters for 2G bioethanol production.

Parameter	Value	Unit
Steam Explosion Pretreatment		
Steam pressure [a]	1.25	MPa
Steam temperature [a]	190	°C
Steam consumption [a]	0.55	kg $kg_{LM, AR}^{-1}$
Hemicellulose hydrolysis [a, b]	70	wt. %
Cellulose hydrolysis [c]	70	wt. %
Lignin solubilisation [b]	0.00	wt. %
Xylose fermentation		
Xylose to ethanol conversion [b]	80	wt. %
Alkaline delignification		
Lignin solubilisation [d]	92.7	wt. %
Enzymatic hydrolysis		
Cellulose hydrolysis [c]	80	wt. %
Hemicellulose hydrolysis [c]	80	wt. %
Filters		
Solids recovery [c]	99.5	wt. %
Soluble solids loss [c]	10	wt. %
Auxiliary operations		
Electricity consumption [b]	-24	kWh $t_{LM, AR}^{-1}$

LM, AR: Lignocellulose material on an as received basis

[a] Ortiz & Oliveira Jr (2014)

[b] Dias, Junqueira, Cavalett, Cunha, Jesus, Rossell, *et al* (2012)

[c] Dias, Junqueira, Rossell, *et al* (2013)

[d] Rocha, Gonçalves, *et al* (2012)

Appendix C: The process model calculations

The process models for sugarcane-bioethanol and soybean-biodiesel were developed in Microsoft Excel and Python. The files can be accessed using the following link:

Click here for the process models and calculations