

Appendix A: System boundary and Aspen Plus component data

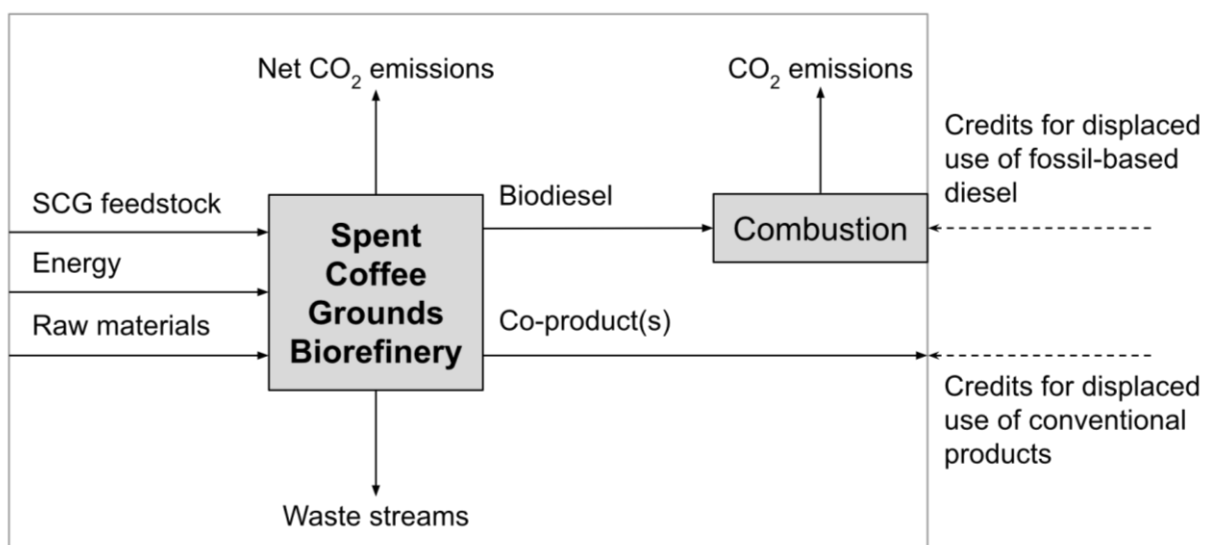


Figure A.1 System boundary for the SCG biorefinery.

Table A.1 Aspen Plus component data and user-defined properties used in process simulation.

Component	Property	Quantity	Units	Reference
CELLULOS	DHSFRM	233200.06	cal/mol	Native Aspen component with specified heat of formation from (Humbird et al., 2011)
HEMI	-	-	-	Hemicellulose, duplicate of CELLULOS
GLUCOSE	-	-	-	Native Aspen component
GALACTOS	-	-	-	Duplicate of GLUCOSE
MANNOSE	-	-	-	Duplicate of GLUCOSE
CELLOB	-	-	-	Cellobiose, used native Aspen component sucrose
LIGNIN	-	-	-	Native Aspen component vanillin
PROTEIN	-	-	-	Native Aspen component glutamic acid
FURFURAL	-	-	-	Native Aspen component
HMF	-	-	-	Native Aspen component
GLUCOLIG	MW	162.14	-	Glucose oligomers. Most properties from GLUCOSE, MW is GLUCOSE minus H ₂ O
ASH	DHFORM	-192875.34	cal/mol	Matches ΔH_c of CELLULOS
CELLULAS	-	-	-	Native Aspen component CaO
BIO	DHSFORM	-17618	cal/mol	From (Humbird et al., 2011)
	DHSFORM	-23200.01	cal/mol	Microbial mass. Native Aspen component C ₃ H ₉ NO ₂ of similar molecular weight as the PHB-microbe molecular structure quoted in (Nieder-Heitmann et al., 2018), DHSFORM from cell mass in (Humbird et al., 2011)
PHB	VSPOLY	70.7	ml/mol	(“Polyhydroxybutyrate,” 2021)
	CPSPO	120.4	kJ/kmol-K	(“Polyhydroxybutyrate,” 2021)
SUCCINIC	-	-	-	Native Aspen component succinic acid

VANILLIN	-	-	-	Native Aspen component vanillin
ACETO-V	-	-	-	Native Aspen component acetovanillone
GUAIACOL	-	-	-	Native Aspen component guaiacol
ACETIC	-	-	-	Native Aspen component acetic acid
FORMIC	-	-	-	Native Aspen component formic acid
NH ₃	-	-	-	Native Aspen component ammonia
NA2SUC	PLXANT/1	-1E20	bar	Native Aspen component disodium succinate forced non-volatile
	DHSFORM	-940	kJ/mol	("Butanedioic acid," 2021)
Ca(OH) ₂	-	-	-	Native Aspen component calcium hydroxide
ARGON	-	-	-	Native Aspen component argon
CAO	-	-	-	Native Aspen component calcium oxide
O ₂	-	-	-	Native Aspen component oxygen
N ₂	-	-	-	Native Aspen component nitrogen
CO ₂	-	-	-	Native Aspen component carbon dioxide
H ₂ O	-	-	-	Native Aspen component water

Note

1. Components of similar physical properties were used to represent compounds whose exact component was not available in the Aspen Plus native databank (Humbird et al., 2011; Trejo-Zárraga et al., 2018).
2. SCG was assumed to have uniform particle size distribution.

Appendix B: SCG feedstock parameters

Table B.1 Parameters used for SCG transport calculations.

Parameter	Unit	Value
SCG delivered to plant	t/day	138.4
Avr return journey distance	km	140.0
Truck payload	t	18.0
Daily number of return journeys	-	8.0
Fuel consumption	miles/gallon	9.5

Table B.2 Parameters for SCG produced in London coffee establishments.

Parameter	Unit	Value	Ref
Green coffee beans imported into UK, 2018 (B_{UK})	t/year	190000	(“The United Kingdom’s market potential for coffee,” 2020)
Proportion of total coffee consumption occurring in coffee establishments (x_{CE})	%	32	(“The United Kingdom’s market potential for coffee,” 2020)
Proportion of total UK coffee establishments found in London (x_{LDN})	%	25.8	(Dinev, 2021)
Moisture content of SCG (x_{WAT})	%	66	(Caetano et al., 2014)

Assumptions

1. All imported coffee beans are consumed.
2. SCG production rate is uniform throughout the year.
3. SCG obtained has been separated from other food wastes.

$$\text{Annual SCG production from London shops} = \frac{B_{UK} \times x_{CE} \times x_{LDN}}{1 - x_{WAT}} \quad \text{Equation (B.1)}$$

Table B.3 Parameters for SCG produced in Nestlé’s instant coffee factory.

Parameter	Unit	Value	Ref
Nestlé factory daily rate of coffee bean processing (B_N)	t/day	108	(“How Is Instant Coffee Made?,” 2021)
Biorefinery’s annual number of operating hours (h)	hours/year	8000	
Moisture content of SCG (x_{WAT})	%	66	(Caetano et al., 2014)

$$\text{Annual SCG production from Nestlé coffee factory} = \frac{B_N}{1 - x_{WAT}} \times \frac{h}{24} \quad \text{Equation (B.2)}$$

Appendix C: Capital expenditure

$$\frac{COST_f}{COST_b} = \left(\frac{SIZE_c}{SIZE_b} \right)^R \quad \text{Equation (C.1)}$$

$$C_r = COST_f \left(\frac{IV_r}{IV_b} \right) \quad \text{Equation (C.2)}$$

$$TCC = 5.03 \times \sum_{i=1}^{n=N_{equip}} C_{r,i} \quad \text{Equation (C.3)}$$

$$CRF = \frac{dr(1+dr)^{PL}}{(1+dr)^{PL}-1} \quad \text{Equation (C.4)}$$

$$CC = TCC \times CRF \quad \text{Equation (C.5)}$$

where

$COST_b$ is the equipment base cost, £;

$COST_f$ is the equipment f.o.b. purchase cost, £;

$SIZE_b$ is the equipment size capacity of the base system;

$SIZE_c$ is the equipment size capacity of the current system as obtained from Aspen Plus simulation results;

R is the scaling exponent;

$C_{r,i}$ is the cost for equipment i in the reference year, £;

IV_r is the CEPCI index value in the reference year;

IV_b is the CEPCI index value in the base year;

TCC is the total capital cost, £;

N_{equip} is the total number of equipment;

CRF is the capital recovery factor;

dr is the discount rate;

PL is the plant lifetime, y;

CC is the annualised capital cost, £/y;

Note

1. F.o.b. purchase cost includes the cost of the equipment and its delivery to the plant.

Appendix D: Operating expenditure

$$\text{Cost of personnel (£/year)} = \text{Number of personnel per shift} \times 5 \text{ shifts} \times 40 \text{ hours/week} \times 52 \text{ weeks/year} \times \text{Hourly wage} \quad \text{Equation (D.1)}$$

$$VAR = C_{RM} + C_U + C_{WT} + C_{CARB} \quad \text{Equation (D.2)}$$

where

VAR is the annual variable operating cost of the plant, £/y;

C_{RM} is the raw material cost, £/y;

C_U is the utilities cost, £/y;

C_{WT} is the waste treatment costs, £/y;

C_{CARB} is the carbon cost based on UK's carbon tax and the plant's net CO₂ emissions, £/y;

Note

1. The hourly wage is taken as £10.90 ("Gross weekly earnings by occupation," 2021)
2. Start-up and shut down costs are excluded.
3. Raw material prices obtained from internet sources ("Alibaba," 2021).
4. Waste treatment costs obtained from Turton et al. (2012)
5. Utility costs obtained from Aspen Plus
6. Carbon tax rate obtained from UK Department for Business, Energy & Industrial Strategy ("Updated short-term traded carbon values used for UK public policy appraisal," 2019).
7. VAR of Configuration II includes growth media costs and the cost of replacing granulated activated carbon and succinic adsorbent 4 times annually (Nieder-Heitmann et al., 2019).

Table D.1

Type of fixed operating cost	Cost estimation	Ref
Laboratory costs	20% of labour costs	(Sorrels et al., 2017)
Supervision	20% of labour costs	(Sorrels et al., 2017)
Plant overheads	22% of labour costs	(Sorrels et al., 2017)
Maintenance	5% of indirect capital costs	(Sadhukhan et al., 2014)
Local taxes and insurance	2% of indirect capital costs	(Sorrels et al., 2017)

where

Indirect capital costs = 1.26 × Total equipment purchase cost (Sadhukhan et al., 2014)

Appendix E: Economic performance indicators

$$EP = h \sum_{i=1}^{i=Np} r_i p_i - CC - OC \quad \text{Equation (E.1)}$$

$$NPV = \sum_{n=0}^{n=PL} \frac{C_f}{(1+dr)^n} \quad \text{Equation (E.2)}$$

where

h is the annual number of operating hours, h;

r_i is the production rate of product i as extracted from Aspen Plus simulation results, kg/h;

p_i is the base unit price of product i , £/kg;

CC is the annualised capital cost, £/y;

OC is the annual operating cost, £/y;

NPV is the net present value, £;

C_f is the cash flow in a particular year, £;

dr is the discount rate

Table E.1 Base unit price of products used for economic analysis.

Product	Market Price (£/kg)	Ref
Biodiesel	0.95	(“Biodiesel prices (SME & FAME),” 2021)
Vanillin	10.80	
Acetovanillone	43.20	
Guaiacol	14.40	
Acetic acid	0.36	(“Alibaba,” 2021)
Formic acid	0.72	
Succinic acid	1.26	
Vanillic acid	10.80	
PHB	8.23	(Nieder-Heitmann et al., 2019)

Appendix F: Net GHG emissions

$$Net\ GHG = E_{RM} + E_D + E_{COMB} + E_{ENERGY} + E_{TRAN} + E_{WT} - CR_E - CR_P \quad \text{Equation (F.1)}$$

where

E_{RM} is the emissions from the manufacturing of the raw materials used, kg CO₂-eq./t SCG;

E_D is the plant net direct CO₂ emissions, kg CO₂-eq./t SCG;

E_{COMB} is the emissions from the combustion of biodiesel produced, kg CO₂-eq./t SCG;

E_{ENERGY} is the emissions due to energy consumed, kg CO₂-eq./t SCG;

E_{TRAN} is the emissions from SCG transport, kg CO₂-eq./t SCG;

E_{WT} is the waste treatment emissions, kg CO₂-eq./t SCG;

CR_E is the emission credit for electricity exported to the grid, kg CO₂-eq./t SCG;

CR_p is the emission credit for the displacement of conventional production of the products generated from SCG, kg CO₂-eq./t SCG

Note

1. Emission credits determined using data on the emissions from the UK grid electricity mix and the displaced products from the Ecoinvent database in CCalC2 software.
2. Emissions from the production of SCG were excluded.
3. E_D is obtained from simulation results by subtracting sum of CO₂ input flowrates from plant CO₂ output flowrate.
4. For Configuration I, E_D excludes emissions generated from the combustion of SCG material as biomass combustion returns the carbon absorbed during plant growth back to the atmosphere (“Fossil vs biogenic CO₂ emissions,” 2021).

Appendix G: Biorefinery Configuration I

Table G.1 Parameters used in oil extraction process model (Najdanovic-Visak et al., 2017).

Parameter	Value
Temperature (°C)	60
Solvent-to-solid ratio (L/kg)	15
Extraction time (hour)	1
Oil extraction yield (kg oil extracted/kg total oil content)	0.96

Table G.2 Parameters used in esterification and transesterification process models (Efthymiopoulos et al., 2018; Hochegger et al., 2019; Saratale et al., 2020).

Parameter	Esterification	Transesterification
Temperature (°C)	60	60
Methanol-to-lipid molar ratio	40	6
Catalyst loading (wt% lipid)	2	1
Reaction time (hour)	0.5	1
Biodiesel yield (kg biodiesel/kg lipid)	0.88	0.9

Note

1. Lipids refer to FFA for esterification and triglyceride for transesterification.

Table G.3 Key Aspen process models used in Configuration I.

Aspen ID	Aspen Model	Process Unit Description	Temp (°C)	Pres (bar)	Other Specifications or notes
OILEXTR	Mixer	Oil Extraction	60.05	1	Extracted oil content modelled as liquid phase in input
EST	RStoic	Esterification of FFA	60	1	$\text{FFA} + \text{METHANOL} \rightarrow \text{BDIESEL} + \text{H}_2\text{O}$
TRAN	RStoic	Transesterification	60	1	$\text{TRIOLEIN} + 3 \text{METHANOL} \rightarrow 3 \text{BDIESEL} + \text{GLYCEROL}$ $2 \text{NaOH} + \text{H}_2\text{SO}_4 \rightarrow 2 \text{H}_2\text{O} + \text{Na}_2\text{SO}_4$
NEUTR	RStoic	Neutralisation	40	1	$2 \text{NaOH} + \text{H}_2\text{SO}_4 \rightarrow 2 \text{H}_2\text{O} + \text{Na}_2\text{SO}_4$
COMBUST	RStoic	Combustion of defatted SCG and organic waste streams	500	1	$\text{CELLU} + 6 \text{O}_2 \rightarrow 6 \text{CO}_2 + 5 \text{H}_2\text{O}$ $2 \text{LIGNIN} + 17 \text{O}_2 \rightarrow 16 \text{CO}_2 + 8 \text{H}_2\text{O}$ $2 \text{CAFFEINE} + 19 \text{O}_2 \rightarrow 16 \text{CO}_2 + 10 \text{H}_2\text{O} + 4 \text{N}_2$ $4 \text{AMINACID} + 21 \text{O}_2 \rightarrow 20 \text{CO}_2 + 18 \text{H}_2\text{O} + 2 \text{N}_2$ $\text{CAFFEIC} + 9 \text{O}_2 \rightarrow 4 \text{H}_2\text{O} + 9 \text{CO}_2$ $\text{TRIOLEIN} + 80 \text{O}_2 \rightarrow 57 \text{CO}_2 + 52 \text{H}_2\text{O}$ $\text{BDIESEL} + 27 \text{O}_2 \rightarrow 19 \text{CO}_2 + 18 \text{H}_2\text{O}$ $2 \text{GLYCEROL} + 7 \text{O}_2 \rightarrow 6 \text{CO}_2 + 8 \text{H}_2\text{O}$ $2 \text{METHANOL} + 3 \text{O}_2 \rightarrow 2 \text{CO}_2 + 4 \text{H}_2\text{O}$ $2 \text{HEXANE} + 19 \text{O}_2 \rightarrow 14 \text{H}_2\text{O} + 12 \text{CO}_2$ $2 \text{FFA} + 51 \text{O}_2 \rightarrow 36 \text{CO}_2 + 34 \text{H}_2\text{O}$

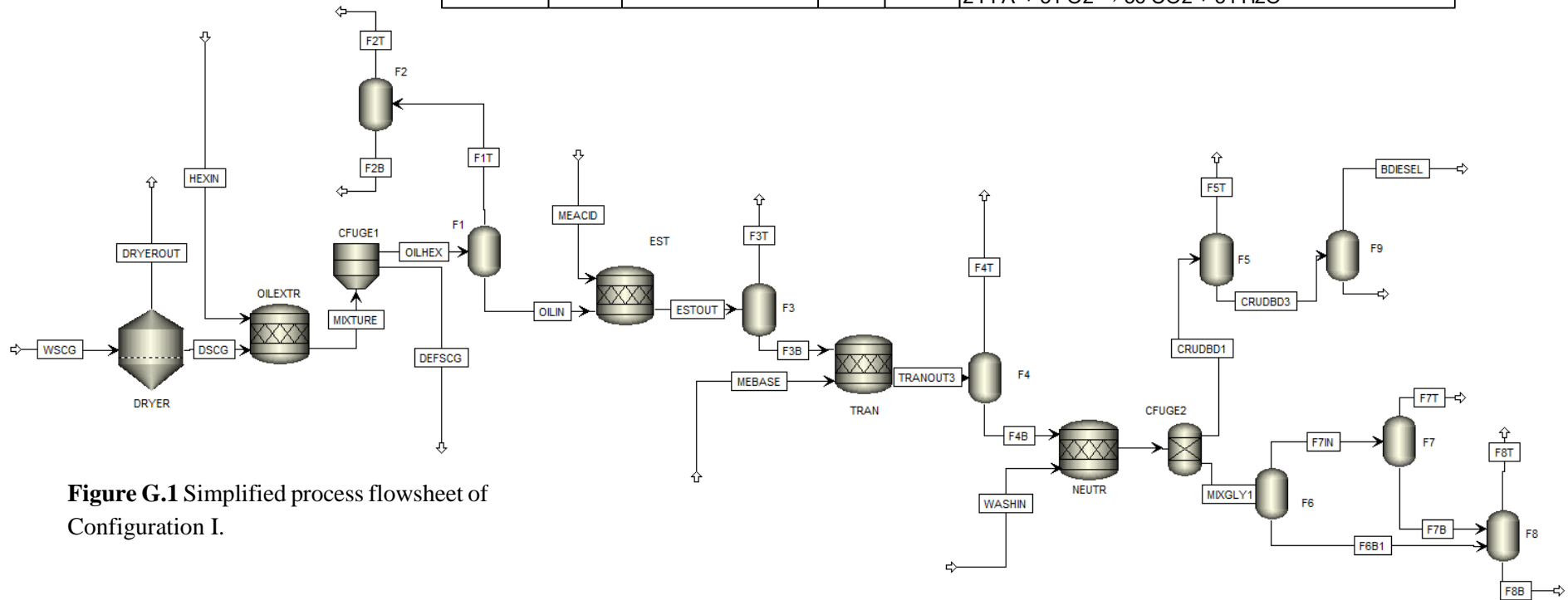


Figure G.1 Simplified process flowsheet of Configuration I.

Table G.4 Stream table for Configuration I using Scenario A parameters.

Stream ID	WSCG	DSCG	HEXIN	MIXTURE	DEFSCG	OILHEX	OILIN	MEACID	ESTOUT	F3B	MEBASE	TRANOUT3	F4B	WASHIN	NEUTPROD	CRUDBD1	CRUDBD3	BDIESEL
Temp (°C)	20.0	60.1	60.1	60.1	60.1	60.1	80.0	60.0	60.0	120.0	60.0	60.0	162.0	40.0	40.0	40.0	166.9	30.2
Pres (bar)	1.0	1.0	1.0	1.0	1.0	1.0	0.1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.1	1.0
Mass flow (kg/h)																		
<i>MIXED Substream</i>																		
H2O	3806.2							37.7	41.5	0.2	5.9	6.6	0.9	76.7	78.5	3.1	0.0	0.0
TRIOLEIN				214.7		214.7	214.7		214.7	214.7	0.0	21.5	21.5	0.0	21.5	0.9	0.9	0.0
HEXANE			19476.3	19476.3		19476.3	1.5	13.9	15.3	0.4	2.1	2.5	0.2	0.0	0.2	0.2	0.0	0.0
METHANOL								302.4	295.7	1.1	46.9	27.0	0.8	0.0	0.8	0.8	0.0	0.0
BDIESEL								0.7	62.3	62.1	0.1	256.3	255.6	0.3	255.9	245.7	243.0	242.4
GLYCEROL								0.9	0.9	0.6	0.1	20.8	20.0	0.0	20.0	0.8	0.0	0.0
NAOH											3.3	2.2	2.2					
H2SO4								1.3	1.3	1.3	0.0			2.7				
FFA			1.2	70.2		70.2	66.7	0.0	8.0	8.0	0.0	8.0	8.0	0.0	8.0	0.3	0.3	0.3
NA2SO4												1.9	1.9		5.8	0.2	0.2	
ARGON																		
<i>CISOLID Substream</i>																		
CAO	39.2	39.2		39.2	39.2													
AMINACID	209.8	209.8		209.8	209.8													
CAFFEINE	0.4	0.4		0.4	0.4													
LIGNIN	529.4	529.4		529.4	529.4													
CELLU(S)	838.8	838.8		838.8	838.8													
TRIO(S)	222.5	222.5		7.9	7.9													
FFA(S)	71.6	71.6		2.5	2.5													
CAFFEIC	49.0	49.0		49.0	49.0													
Total flowrate (kg/h)	5767.0	1960.8	19477.5	21438.3	1677.1	19761.2	282.8	356.9	639.7	288.4	58.4	346.8	311.1	79.8	390.9	252.1	244.4	242.8

*Note that hemicellulose weight is included in cellulose component CELLU(S)

Appendix H: Biorefinery Configuration II

Table H.1 Key Aspen process models used in Configuration II.

Aspen ID	Aspen Model	Process Unit Description	Temp (°C)	Pres (bar)	Other Specifications
ORGP	RStoic	Organosolv	161	1	Dissolving of lignin modelled as lignin input in aqueous phase FFA + CH ₃ OH → Biodiesel + H ₂ O
TRAN	RStoic	Transesterification	60	1	Triolein + 3 CH ₃ OH → 3 Biodiesel + C ₃ H ₈ O ₃
BDNEUT	RStoic	Neutralisation	40	1	2 NaOH + H ₂ SO ₄ → 2 H ₂ O + Na ₂ SO ₄
PRECIP	RStoic	Lignin Precipitation	34	0.1	LIGNIN → LIGN(S)
OXI	RStoic	Oxidative depolymerisation of lignin [19]	160	8	LIGN + 3.235 O ₂ → 1.09 VANILLIN + 1.28 CO ₂ + 2.64 H ₂ O LIGN + 1.78 O ₂ → 0.62 CO ₂ + 1.64 H ₂ O + 1.34 GUAIACOL LIGN + 4.58 O ₂ → 0.99 VANILLIC + 2.08 CO ₂ + 3.04 H ₂ O LIGN + 10.7 O ₂ → 3.6 FORMIC + 6.4 CO ₂ + 3.4 H ₂ O LIGN + 6.96 O ₂ → 2.77 ACETIC + 4.46 CO ₂ + 1.46 H ₂ O LIGN + 2.5 O ₂ → ACETO-V + 2 H ₂ O + CO ₂
MEM	Sep	Membrane separation of organic compounds			Split fraction; Outlet Stream: ORGANIC, Substream: MIXED GUAIACOL, ACETIC, FORMIC, VANILLIN, SUCCINIC, VANILLIC, ACETO-V, METHANOL = 1, Other components = 0
DAP	RStoic	Dilute acid pretreatment of hemicellulose [50] [49]	163	1	H ₂ O + HEMI(S)(CISOLID) → GALACTOS(MIXED) CELLU → HMF + 2 H ₂ O 5 HEMI → 6 FURFURAL + 13 H ₂ O CELLU + H ₂ O → 3 ACETIC CELLU + H ₂ O → GLUCOSE 2 CELLU + H ₂ O → CELLOB Galactose reactions identical to all mannose reactions
EH	RStoic	Enzymatic pretreatment	48	1	CELLU + H ₂ O → GLUCOSE CELLU → GLUCOLIG
PHBG	RStoic	PHB Growth Reactor	30	1	GLUCOSE + 1.02 NH ₃ + 2.43 O ₂ → 1.02 BIO + 2.94 CO ₂ + 2.94 H ₂ O
PHBS	RStoic	PHB Seed reactor	30	1	GLUCOSE + 1.5 O ₂ → PHB + 2 CO ₂ + 3 H ₂ O GLUCOSE + 4 O ₂ → ACETIC + 4 CO ₂ + 4 H ₂ O GLUCOSE + 1.02 NH ₃ + 2.43 O ₂ → 1.02 BIO + 2.94 CO ₂ + 2.94 H ₂ O GLUCOSE + 6 O ₂ → 6 H ₂ O + 6 CO ₂
BLEND	RStoic	Blending tank to lyse cells	30	1	No reaction modelled- cell biomass considered to be lysed into aqueous form and thus removed in CFUGE6
GAC	Sep	Adsorption column [22]			Split fraction; Outlet Stream: TOXINOUT, Substream: MIXED H ₂ O, NAOH, H ₂ SO ₄ = 0.00459, FURFURAL = 0.7, HMF = 1 Other components = 0
NEUT	RStoic	Neutralisation of acid	38	1	H ₂ SO ₄ + CA(OH) ₂ → 2 H ₂ O + CASO ₄
SASEED	RStoic	SA Seed reactor	38	1	GLUCOSE + 1.71429 NH ₃ → 1.71429 BIO + 0.857143 CO ₂ + 0.857143 H ₂ O MANNOSE + 1.71429 NH ₃ → 1.71429 BIO + 0.857143 CO ₂ + 0.857143 H ₂ O Galactose reactions identical to all mannose reactions
SAFERM	RStoic	SA Fermentor	38	1	GLUCOSE + 1.71429 NH ₃ → 1.71429 BIO + 0.857143 CO ₂ + 0.857143 H ₂ O MANNOSE + 1.71429 NH ₃ → 1.71429 BIO + 0.857143 CO ₂ + 0.857143 H ₂ O GLUCOSE + 0.8571 CO ₂ → 1.7142 SUCCINIC + 0.8571 H ₂ O 2 GLUCOSE + 3 CO ₂ → 3 SUCCINIC + 3 FORMIC 3 GLUCOSE + 2 CO ₂ → 4 SUCCINIC + 2 ACETIC + 2 H ₂ O 5.83333 MANNOSE + 5 CO ₂ → 10 SUCCINIC + 5 H ₂ O CELLOB + CO ₂ → 2 SUCCINIC + 2.5 ACETIC 2.5 MANNOSE + 2 CO ₂ → 4 SUCCINIC + 0.5 ACETIC + 2 H ₂ O Galactose reactions identical to all mannose reactions
SA-EXTRAC	Sep	Adsorption tower with resin NERCB09			Split fraction; Outlet Stream: SAMIX1, Substream: MIXED ACETIC = 0.069, FORMIC = 1, SUCCINIC = 0.96, NAOH = 1 Other components = 0
PRECP	RStoic	Selective precipitation of sodium sulfate	70	1	2 NAOH + Succinic Acid → Sodium Succinate + 2 H ₂ O Sodium Succinate + H ₂ SO ₄ → Sodium Sulfate + Succinic Acid

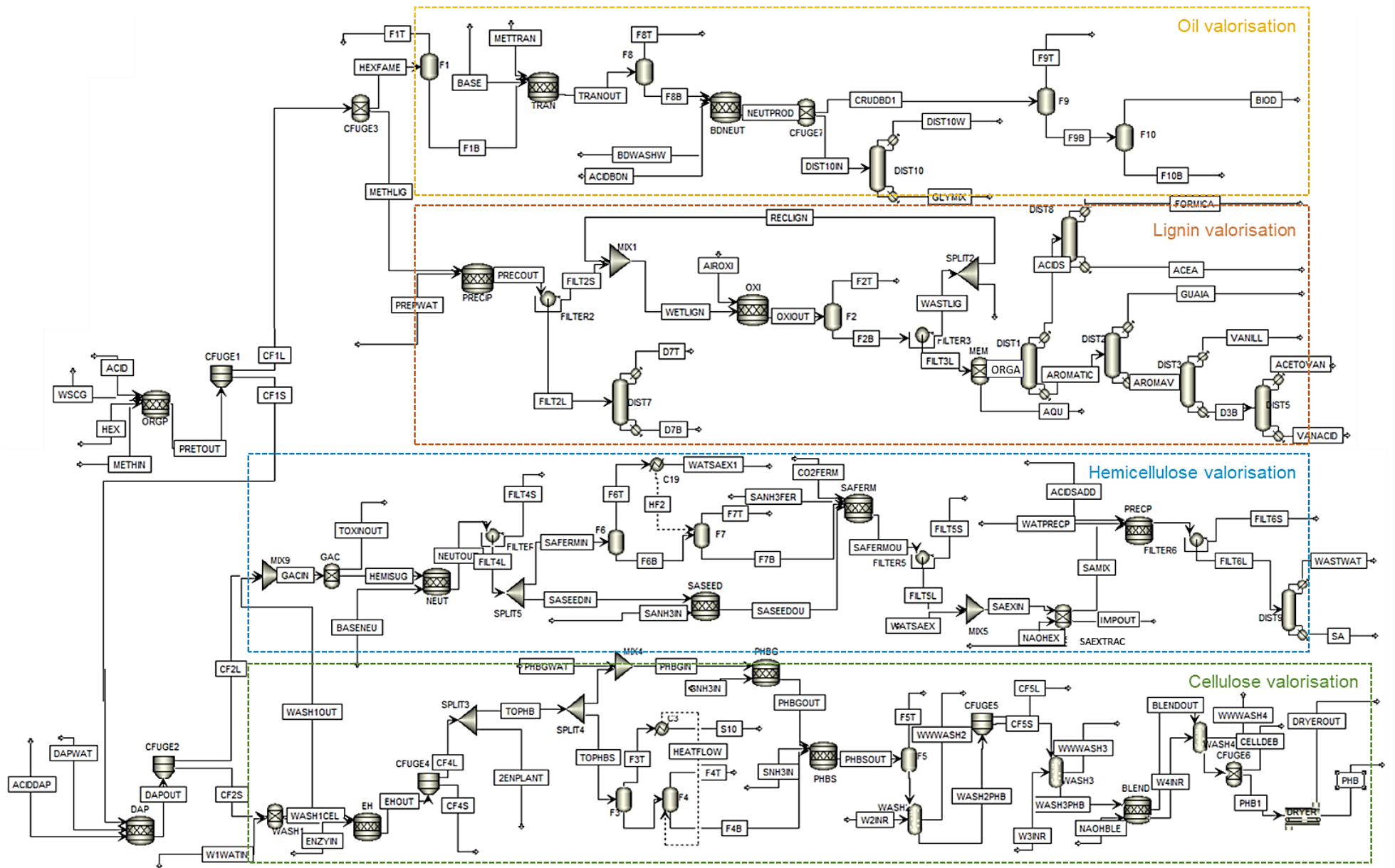


Figure H.1 Simplified process flowsheet of Configuration II.

Table H.2 Stream table for Configuration II using Scenario D parameters.

Stream ID	WSCG	PRETOUT	DAPOUT	WASH1CEL	ENZYIN	EHOUT	PHBGIN	PHBGOUT	F4B	PHBSOUT	WASH3PHB	BLENDOUT	PHB	SASEEDIN	SASEEDOU	F7B	SAFERMOU	SAMIX	
Temp (°C)	20.0	161.0	163.0	40.0	48.0	48.0	30.0	30.0	105.0	30.0	30.0	30.0	100.0	38.0	38.0	100.3	38.0	37.0	
Pres (bar)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	
Mass flow (kg/h)																			
<i>MIXED Substream</i>																			
H2O	3806.2	3845.9	13803.6	2900.9		2882.0	812.0	815.4	85.0	954.9	1509.0	3021.5		1411.1	1411.3	2335.3	3778.7		
TRIOLEIN		173.6																	
HEXANE		6102.1																	
METHANOL		7315.4																	
BDIESEL		47.3																	
CAFFEINE		0.4																	
GLUCOSE			11.5			188.9	16.6	4.9	157.8					1.1	1.0	10.3	1.2		
NAOH											11.6	23.7						253.2	
O2							5.0												
CO2								8.4	0.0	118.0	0.5	0.5			0.6				
H2SO4		1216.5	135.8																
FFA		11.2																	
CAFFEIC		49.0																	
LIGNIN		296.5																	
ACETIC			19.3							0.1				1.9	1.9	1.9	15.2	1.1	
SUCCINIC																		389.4	373.8
MANNOSE			307.5											30.8	29.4	276.8	118.8		
GALACTOS			307.5											30.8	29.4	276.8	118.8		
CELLOB			0.1													0.1			
FURFURAL			25.7											0.8	0.8	0.1	0.9		
HMF			0.3																
GLUCOLIG						7.5	0.7	0.7	6.2	6.9	0.4	0.4							
CELLULAS					3.7	3.7	0.3	0.3	3.1	3.4	0.2	0.2							
NH3							1.1												
<i>CISOLID Substream</i>																			
CAO	39.2	39.2	39.2	39.2		39.2													
AMINACID	209.8	209.8	209.8	209.8		209.8													
CAFFEINE	0.4																		
LIGNIN	529.4	232.9	232.9	232.9		232.9													
CELLU(S)	214.7	214.7	186.5	186.5		8.9													
HEMI(S)	624.1	624.1	34.3	34.3		34.3													
BIO(S)									6.0	30.5	30.5	30.5	0.7		2.4	0.0	26.0		
PHB(S)										45.6	45.6	45.6	44.2		0.0	0.0	0.0		
TRIO(S)	222.5	49.0	49.0	49.0		49.0													
FFA(S)	71.6	15.7	15.7	15.7		15.7													
CAFFEIC	49.0																		
Total flowrate (kg/h)	5767.0	20443.3	15378.9	3668.4	3.7	3672.1	835.7	835.7	252.2	1159.4	1597.8	3122.4	44.9	1476.4	1476.9	2901.4	4448.9	628.0	

Table H.3 Stream table for Configuration II using Scenario D parameters (continued).

Stream ID	FILT6L	SA	METHLIG	WETLIGN	OXIOUT	ORGA	ACIDS	AROMATIC	FORMICA	ACEA	GUAIA	VANILL	ACETOVAN	VANACID	F1B	TRANOUT	CRUDBD1	BIOD
Temp (°C)	70.0	30.0	43.0	160.0	160.0	35.0	41.5	193.6	15.1	30.2	30.1	30.2	30.2	30.2	75.0	60.0	40.0	30.2
Pres (bar)	1.0	1.0	1.0	8.0	8.0	3.0	0.1	0.1	1.0	1.0	1.0	1.0	1.0	1.0	0.1	1.0	1.0	1.0
Mass flow (kg/h)																		
<i>MIXED Substream</i>																		
H2O	554.5	1.8	3845.9		83.2													2.5
TRIOLEIN															173.6	17.4		0.7
HEXANE															3.5	20.1		2.6
METHANOL			7315.4															0.7
BDIESEL															46.9	204.2	195.6	193.2
GLYCEROL																		0.6
NAOH																		1.7
O2																		
N2					1271.1													
CO2					308.1													
H2SO4			1216.5															
FFA															11.2	11.2		0.4
ARGON					23.2													
NA2SO4																		0.1
LIGNIN			296.5															
CAFFEIC			49.0															
CAFFEINE			0.4															
GUAIACOL					22.7	22.7		22.7			22.2	0.5						
ACETIC	1.7				46.1	40.8	40.8		0.8	40.0								
FORMIC					126.4	103.1	103.1		102.3	0.8								
VANILLIN					42.4	42.4		42.4			0.2	42.2						
SUCCINIC	276.6	274.8																
VANILLIC					32.9	32.9		32.9					0.1	32.7				
ACETO-V					10.2	10.2		10.2				0.5	9.6	0.1				
FURFURAL	0.3																	
<i>CISOLID Substream</i>																		
LIGNIN				3388.4	3107.4													
Total flowrate (kg/h)	833.1	276.6	12723.7	3388.4	5073.6	252.0	143.9	108.1	103.1	40.8	22.4	43.2	9.6	32.8	235.1	286.4	203.3	193.7

Appendix I: Economic assessment results

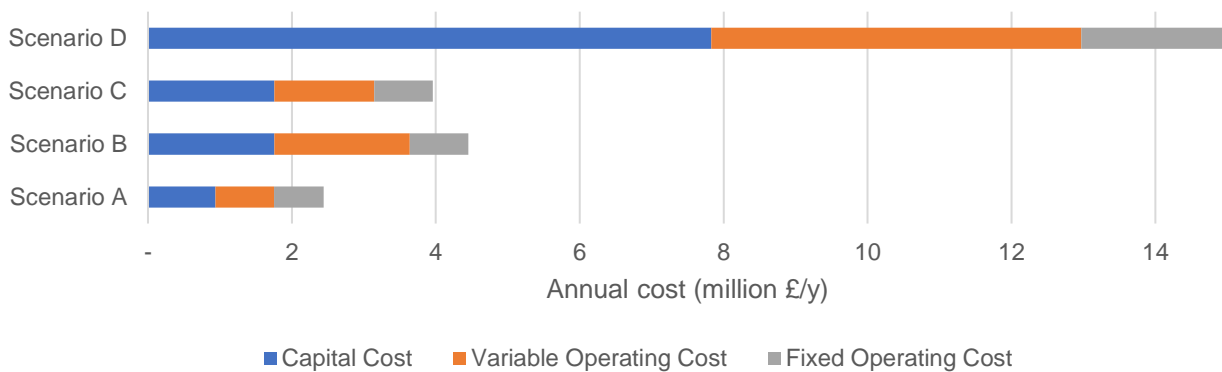


Figure I.1 Classification of costs by type.

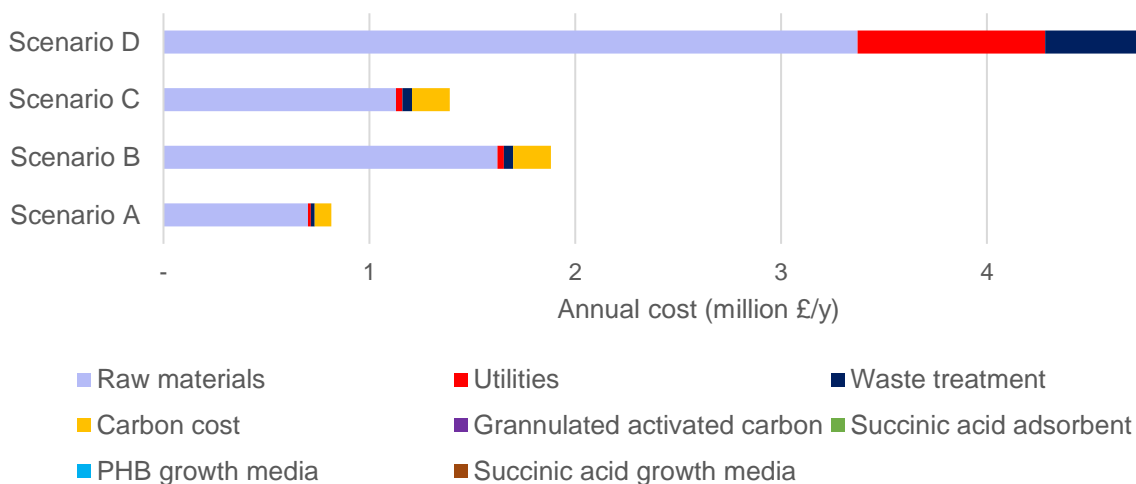
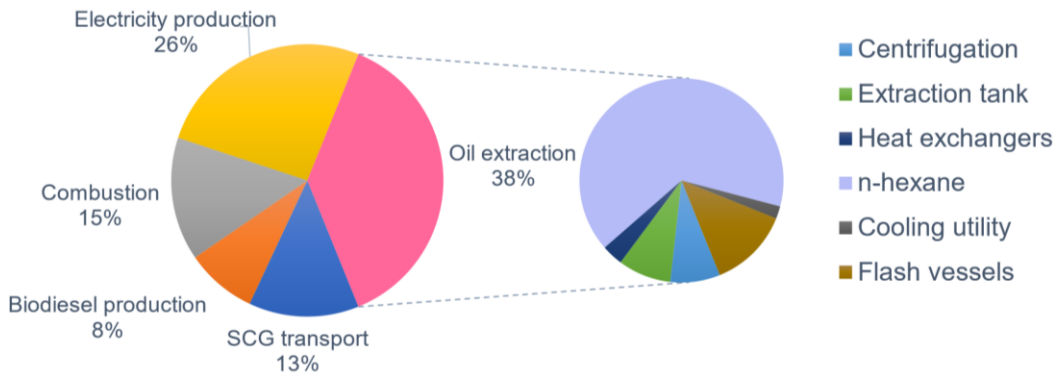


Figure I.2 Classification of variable operating costs.

Scenario A



Scenario D

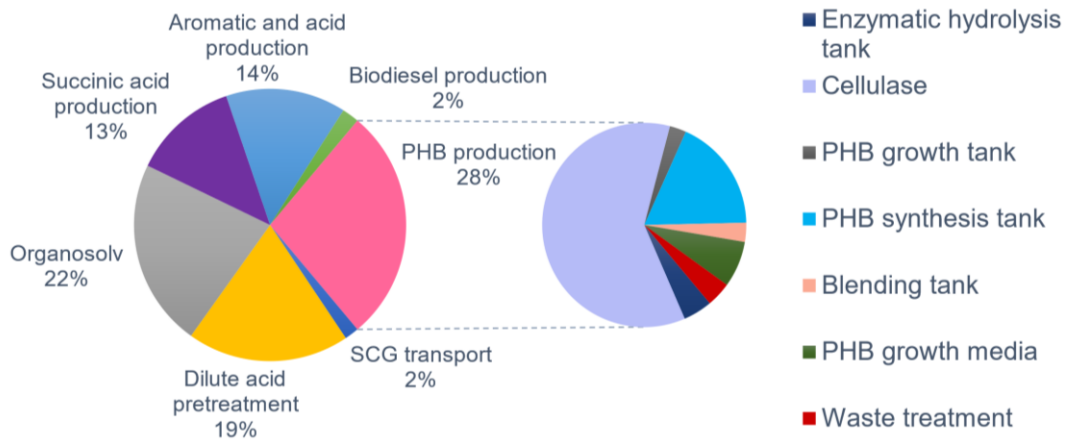


Figure I.3 Classification of costs by process.