# Introduction

Beer production constitutes one of the largest sectors of the global beverage industry. After the malting, milling, and mashing of the initial barley grains, the wort filtration generates an insoluble solid fraction known as brewer’s spent grains (BSG), which includes the husk and outer layers of the seeds. It represents the most abundant by-product of the brewing industry, accounting for up to 85% of the total waste and yielding approximately 20 kg of BSG per 100 L of beer produced.

The chemical composition of BSG depends on the type of fruit, harvest time, technology, and brewing process parameters, although it primarily consists of a lignocellulosic fibrous material with a high protein content. The fiber component is largely made up of hemicellulose, cellulose, and lignin; while monosaccharides (glucose, xylose, and arabinose), lipids, amino acids, and phenolic compounds are also present. Regarding moisture content, it hovers around 80%.

Currently, BSG is predominantly used for animal feed or disposed of in environmentally undesirable ways in landfills. However, its abundant availability and characteristic physicochemical properties provide the opportunity to explore new biotechnological approaches for valorization toward high-value-added products. In this context, the present case study explores some of the potential production routes of microbial fermentation to ethanol, extraction of proteins, and anaerobic digestion to biogas and compost from BSG.

# Define the general data system

Table 1 includes the initial information that must be defined in the software regarding plant production, capital cost calculations, and possible heat recovery systems. It should be noted that the facility's capacity was estimated to represent the amount of BSG processed by the Danish company Agrain, whose objective is to produce brewery-based flour.

Table 1. Definition of general system parameters

|  |  |  |
| --- | --- | --- |
|  | **Parameter** | **Value** |
| **Specific production** | Load type | Substrate |
| Main product / Substrate | BSG |
| Substrate load (t/y) | 4800 |
| **General CAPEX**  **parameters** | Operating hours (h/y) | 8000 |
| Year of Study | 2020 |
| Interest rate (-) | 0.05 |
| Detail level of linearization of CAPEX | Real |
| Indirect Cost Factor (-) | 1.44 |
| Direct Cost Factor (-) | 2.60 |
| **Heat pump parameters** | Heat pump switch | No |

# Define the chemicals compounds

Table 2 lists the compounds involved in the three proposed production routes, also providing heat capacity and molecular weight data when necessary.

Table 2. Compounds required for the production systems proposed

|  |  |  |
| --- | --- | --- |
| **Component** | **Heat capacity (kJ/kg·K)** | **Molecular weight (g/mol)** |
| Acetyl groups | – | – |
| Ash | – | – |
| Cellulose | – | – |
| Extractives | – | – |
| Hemicellulose | – | – |
| Lignin | – | – |
| Lipids | – | – |
| Phenolics | – | – |
| Proteins | – | – |
| Starch | – | – |
| NaOH | 1.40 | 40.00 |
| H2O | 4.18 | 18.01 |
| H2SO4 | 3.60 | 98.08 |
| Enzymes | – | – |
| Sugar | – | – |
| Biomass | – | – |
| CH4 | 2.22 | 16.04 |
| CO2 | 0.84 | 44.01 |
| O2 | 0.92 | 32.00 |
| N2 | 1.04 | 28.01 |
| EtOH | 2.44 | 46.07 |
| Biogas | – | – |
| Compost | – | – |

# Define the reactions

Table 3 and Table 4 specify the mass balances of the syntheses that take place in the stoichiometric reaction units for the biogas and ethanol production routes, respectively.

Table 3. Reactions involved in anaerobic digestion and cogeneration plant

|  |  |
| --- | --- |
| **Reaction name** | **Reaction equation** |
| Acetyl groups DA | -1 Acetyl groups → 0.33 CH4 + 0.57 CO2 + 0.1 Biomass |
| Cellulose DA | -1 Cellulose → 0.2 CH4 + 0.7 CO2 + 0.1 Biomass |
| Hemicellulose DA | -1 Hemicellulose → 0.15 CH4 + 0.75 CO2 + 0.1 Biomass |
| Lipids DA | -1 Lipids → 0.56 CH4 + 0.34 CO2 + 0.1 Biomass |
| Proteins DA | -1 Proteins → 0.33 CH4 + 0.57 CO2 + 0.1 Biomass |
| Starch DA | -1 Starch → 0.25 CH4 + 0.65 CO2 + 0.1 Biomass |
| CHP | -1 CH4 – 4 O2 → 2.75 CO2 + 2.25 H2O |

Table 4. Reactions involved in auto-enzymatic hydrolysis and fermentation to produce ethanol

|  |  |
| --- | --- |
| **Reaction name** | **Reaction equation** |
| Cellulose auto-enzymatic hydrolysis | -1 Cellulose → 0.7 Sugar + 0.3 Cellulose |
| Hemicellulose auto-enzymatic hydrolysis | -1 Hemicellulose → 0.7 Sugar + 0.3 Hemicellulose |
| Starch auto-enzymatic hydrolysis | -1 Starch → 0.7 Sugar + 0.3 Starch |
| Ethanol fermentation | -1 Sugar → 0.47 EtOH + 0.45 CO2 + 0.08 Sugar |

# Define the utilities

Table 5 shows the costs and CO2 emissions associated with the electricity or heat exchange utilities used in the processes, also including the typical temperature ranges for the latter case.

Table 5. Definition of system utilities

|  |  |  |  |
| --- | --- | --- | --- |
| **Utility**  **data** | **Parameter** | **Costs (€/MWh)** | **CO2 emissions (t/MWh)** |
| Electricity | 120 | 0.33 |
| Heat | – | 0.24 |
| Chilling | 35 | 0.10 |
| **Temperature data** | **Parameter** | **Temperature (ºC)** | **Costs (€/MWh)** |
| Superheated steam | 140 | 29 |
| High pressure steam | 110 | 29 |
| Medium pressure steam | 100 | 29 |
| Low pressure steam | 95 | 29 |
| Cooling water | 15 | 29 |

# Inputs information for the superstructure mapping

Table 6, Table 7, Table 8, Table 9, Table 10 and Table 11 provide the prices and composition fractions for each of the inputs required to produce proteins, ethanol, and biogas.

Table 6. Information to define BSG input

|  |  |  |
| --- | --- | --- |
| **Source name** | BSG | |
| **Cost input (€/t)** | -59 | |
| **Components** | **Component name** | **Composition fraction** |
| Acetyl groups | 0.01 |
| Ash | 0.03 |
| Cellulose | 0.15 |
| Extractives | 0.06 |
| Hemicellulose | 0.21 |
| Lignin | 0.15 |
| Lipids | 0.06 |
| Phenolics | 0.01 |
| Proteins | 0.17 |
| Starch | 0.15 |

Table 7. Information to define NaOH solution input

|  |  |  |
| --- | --- | --- |
| **Source name** | NaOH (w) | |
| **Cost input (€/t)** | 6.95 | |
| **Components** | **Component name** | **Composition fraction** |
| H2O | 0.99 |
| NaOH | 0.01 |

Table 8. Information to define H2SO4 solution input

|  |  |  |
| --- | --- | --- |
| **Source name** | H2SO4 (w) | |
| **Cost input (€/t)** | 14 | |
| **Components** | **Component name** | **Composition fraction** |
| H2O | 0.91 |
| H2SO4 | 0.09 |

Table 9. Information to define enzymes input

|  |  |  |
| --- | --- | --- |
| **Source name** | Enzymes | |
| **Cost input (€/t)** | 3036 | |
| **Components** | **Component name** | **Composition fraction** |
| Enzymes | 1 |

Table 10. Information to define air input

|  |  |  |
| --- | --- | --- |
| **Source name** | Air | |
| **Cost input (€/t)** | 0 | |
| **Components** | **Component name** | **Composition fraction** |
| O2 | 0.21 |
| N2 | 0.79 |

Table 11. Information to define water input

|  |  |  |
| --- | --- | --- |
| **Source name** | Water | |
| **Cost input (€/t)** | 1.9 | |
| **Components** | **Component name** | **Composition fraction** |
| H2O | 1 |

It is worth mentioning that each input has been assigned a name that will be used to refer to them in the unit operations of the routes in which they are involved. Additionally, in Table 6 a gate fee of 59 €/t of BSG was applied, which represents the cost of avoiding landfill management of the waste in Denmark.

# Outputs information for the superstructure mapping

Table 12 shows the sales prices of the main products obtained in the proposed production routes.

Table 12. Information to define the main products of the processes

|  |  |  |
| --- | --- | --- |
| **Product name** | **Price output Input (€/t)** | **Product Type** |
| Proteins | 1500 | Main product |
| Ethanol | 1100 | Main product |
| Biogas | 555 | Main product |
| Compost | 10 | Main product |

# Pretreatment unit operations for the routes

Grinding BSG reduces the particle size of the solid and improves accessibility to its internal matrix components, increasing efficiency in fermentation or extraction processes. Therefore, Table 13 includes the data necessary to configure this pretreatment unit operation in the software.

Table 13. Definition of the grinding unit

|  |  |
| --- | --- |
| **Grinding** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 25 |
| **Cost related parameters** | |
| Reference flow type | Entering mass flow |
| Reference flow (t/h) | 250 |
| Components | Solids of the input streams |
| Reference cost (M€) | 0.255 |
| Reference Year | 2017 |
| Exponent | 0.60 |
| **Utility requirements – Electricity requirements** | |
| Reference flow type | Entering mass flow |
| Energy consumption (MWh/t) | 0.016 |
| Components | Solids of the input streams |
| **Separation efficiency** | |
| Separation information | All components enter the next unit |

# Rute from BSG to proteins

Table 14, Table 15 and Table 16 provide the data required to represent the extraction, centrifugation and drying units that can be combined to achieve the production of proteins from dried and ground BSG, correspondingly.

Table 14. Definition of the extraction unit for proteins production (Part 1)

|  |  |
| --- | --- |
| **Alkali-acid extraction** | |
| **Inputs** | |
| Source name | NaOH (w); H2SO4 (w) |

Table 14. Definition of the extraction unit for proteins production (Part 2)

|  |  |  |
| --- | --- | --- |
| **Alkali-acid solid-liquid extraction** | | |
| **General parameters** | | |
| Parameters | Value | |
| Temperature in (ºC) | 25 | |
| Temperature out (ºC) | 121 | |
| **Cost related parameters** | | |
| Reference flow type | Entering mass flow | |
| Reference flow (t/h) | 3 | |
| Components | All components of the input streams | |
| Reference cost (M€) | 0.073 | |
| Reference Year | 2006 | |
| Exponent | 0.53 | |
| **Utility requirements – Electricity requirements** | | |
| Reference flow type | Entering mass flow | |
| Energy consumption (MWh/t) | 0.00049 | |
| Components | All components of the input streams | |
| **Heating Requirements** | | |
| Reference flow type | Entering Flow Heat Capacity | |
| Required Cooling / Heating (∆T) | 96 | |
| Components | Liquids of the input streams | |
| **Mixing Coefficients** | | |
| Mixing coefficient | 42.66 | |
| Mixing Table: Reference flow 1 | Reference Flow Type | Entering mass flow |
| Components | H2O; NaOH; H2SO4 |
| Mixing Table: Reference flow 2 | Reference Flow Type | Entering mass flow |
| Components | All components of the BSG |
| **Separation efficiency** | | |
| Separation information | 22% protein recovery | |
| The remaining components all enter the next unit | |

Table 15. Definition of the centrifugation unit for proteins production (Part 1)

|  |  |
| --- | --- |
| **Centrifugation** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 25 |
| **Cost related parameters** | |
| Reference flow type | Entering mass flow |
| Reference flow (t/h) | 7.92 |
| Components | Liquids of the input streams |
| Reference cost (M€) | 0.213 |
| Reference Year | 2006 |
| Exponent | 0.38 |

Table 15. Definition of the centrifugation unit for proteins production (Part 2)

|  |  |
| --- | --- |
| **Centrifugation** | |
| **Utility requirements – Electricity requirements** | |
| Reference flow type | Entering mass flow |
| Energy consumption (MWh/t) | 0.01 |
| Components | Solids of the input streams |
| **Separation efficiency** | |
| Separation information | Liquid stream with dissolved recovered proteins |
| Solid stream with 10% liquid loss |

Table 16. Definition of the drying unit for proteins production

|  |  |
| --- | --- |
| **Drying** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 55 |
| **Cost related parameters** | |
| Reference flow type | Entering mass flow |
| Reference flow (t/h) | 3.6 |
| Components | Liquid that needs to be evaporated |
| Reference cost (M€) | 1.94 |
| Reference Year | 2006 |
| Exponent | 0.42 |
| **Heating Requirements** | |
| Reference flow type | Entering Flow Heat Capacity |
| Required Cooling / Heating (∆T) | 30 |
| Components | Liquids of the input streams |
| **Separation efficiency** | |
| Separation information | Proteins with 5% impurities as final product |

# Rute from BSG to ethanol

Table 17, Table 18, Table 19, Table 20 and Table 21 provide the data required to represent the hydrolysis, fermentation, centrifugation, distillation and dehydration units that can be combined to achieve the production of ethanol from dried and ground BSG, correspondingly.

Table 17. Definition of the hydrolysis unit for ethanol production (Part 1)

|  |  |
| --- | --- |
| **Auto and enzymatic hydrolysis** | |
| **Inputs** | |
| Source names | Water |
| Enzymes |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 50 |

Table 17. Definition of the hydrolysis unit for ethanol production (Part 2)

|  |  |  |
| --- | --- | --- |
| **Auto and enzymatic hydrolysis** | | |
| **Cost related parameters** | | |
| Reference flow type | Entering mass flow | |
| Reference flow (t/h) | 0.03 | |
| Components | All components of the input streams | |
| Reference cost (M€) | 0.073 | |
| Reference Year | 2006 | |
| Exponent | 0.53 | |
| **Utility requirements – Electricity requirements** | | |
| Reference flow type | Entering mass flow | |
| Energy consumption (MWh/t) | 0.00049 | |
| Components | All components of the input streams | |
| **Heating Requirements** | | |
| Reference flow type | Entering Flow Heat Capacity | |
| Required Cooling / Heating (∆T) | 25 | |
| Components | Liquids of the input streams | |
| **Mixing Coefficients** | | |
| Mixing coefficient | 4.02 | |
| Mixing Table: Reference flow 1 | Reference Flow Type | Entering mass flow |
| Components | H2O; Enzymes |
| Mixing Table: Reference flow 2 | Reference Flow Type | Entering mass flow |
| Components | All components of the BSG |
| **Reactions** | | |
| Reaction name | Conversion (%) | Reactant |
| Cellulose auto-enzymatic hydrolysis | 100 | Cellulose |
| Hemicellulose auto-enzymatic hydrolysis | 100 | Hemicellulose |
| Starch auto-enzymatic hydrolysis | 100 | Starch |
| **Separation efficiency** | | |
| Separation information | All components enter the next unit | |

Table 18. Definition of the fermentation unit for ethanol production (Part 1)

|  |  |
| --- | --- |
| **Fermentation** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 50 |
| Temperature out (ºC) | 30 |
| **Cost related parameters** | |
| Reference flow type | Entering mass flow |
| Reference flow (t/h) | 0.21 |
| Components | All components of the input streams |
| Reference cost (M€) | 0.407 |
| Reference Year | 2006 |
| Exponent | 0.53 |

Table 18. Definition of the fermentation unit for ethanol production (Part 2)

|  |  |  |
| --- | --- | --- |
| **Fermentation** | | |
| **Utility requirements – Electricity requirements** | | |
| Reference flow type | Entering mass flow | |
| Energy consumption (MWh/t) | 0.00033 | |
| Components | All components of the input streams | |
| **Heating Requirements** | | |
| Reference flow type | Entering Flow Heat Capacity | |
| Required Cooling / Heating (∆T) | -20 | |
| Components | Liquids of the input streams | |
| **Reactions** | | |
| Reaction name | Conversion (%) | Reactant |
| Ethanol fermentation | 100 | Sugar |
| **Separation efficiency** | | |
| Separation information | Release of the CO2 produced  The remaining components all enter the next unit | |

Table 19. Definition of the centrifugation unit for ethanol production

|  |  |
| --- | --- |
| **Centrifugation** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 30 |
| Temperature out (ºC) | 30 |
| **Cost related parameters** | |
| Reference flow type | Entering mass flow |
| Reference flow (t/h) | 7.92 |
| Components | Liquids of the input streams |
| Reference cost (M€) | 0.213 |
| Reference Year | 2006 |
| Exponent | 0.38 |
| **Utility requirements – Electricity requirements** | |
| Reference flow type | Entering mass flow |
| Energy consumption (MWh/t) | 0.01 |
| Components | Solids of the input streams |
| **Separation efficiency** | |
| Separation information | Liquid stream with the main product |
| Solid stream with 10% liquid loss |

Table 20. Definition of the distillation unit for ethanol production (Part 1)

|  |  |
| --- | --- |
| **Distillation** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 30 |
| Temperature out (ºC) | 82 |

Table 20. Definition of the distillation unit for ethanol production (Part 2)

|  |  |
| --- | --- |
| **Distillation** | |
| **Cost related parameters** | |
| Reference flow type | Entering mass flow |
| Reference flow (t/h) | 123.86 |
| Components | All components of the input streams |
| Reference cost (M€) | 0.60 |
| Reference Year | 2008 |
| Exponent | 0.60 |
| **Utility requirements – Electricity requirements** | |
| Reference flow type | Entering mass flow |
| Energy consumption (MWh/t) | 0.0000153 |
| Components | All components of the input streams |
| **Heating Requirements** | |
| Reference flow type | Entering mass flow |
| Required Cooling / Heating (MWh/t) | 0.21 |
| Components | All components of the input streams |
| **Separation efficiency** | |
| Separation information | EtOH 90% of mass purity in distillate (96% recovery) |

Table 21. Definition of the dehydration unit for ethanol production

|  |  |  |
| --- | --- | --- |
| **Dehydration** | | |
| **Inputs** | | |
| Source names | Air | |
| **General parameters** | | |
| Parameters | Value | |
| Temperature in (ºC) | 25 | |
| Temperature out (ºC) | 25 | |
| **Cost related parameters** | | |
| Reference flow type | Entering mass flow | |
| Reference flow (t/h) | 0.86 | |
| Components | All components of the input streams | |
| Reference cost (M€) | 0.271 | |
| Reference Year | 2008 | |
| Exponent | 0.60 | |
| **Mixing Coefficients** | | |
| Mixing coefficient | 138.11 | |
| Mixing Table: Reference flow 1 | Reference Flow Type | Entering mass flow |
| Components | H2O; EtOH |
| Mixing Table: Reference flow 2 | Reference Flow Type | Entering mass flow |
| Components | O2; N2 |
| **Separation efficiency** | | |
| Separation information | EtOH with 1% impurities as final product | |

# Rute from BSG to biogas

Table 22, Table 23, Table 24 and Table 25 provide the data required to represent the anaerobic digestion, composting, bioupgrading or Combined Heat and Power (CHP) units that can be combined to achieve the production of compost, biogas or heat and power from dried and ground BSG, correspondingly.

Table 22. Definition of the anaerobic digestion unit for biogas / heat and power / compost production

|  |  |  |
| --- | --- | --- |
| **Thermophilic anaerobic digestion** | | |
| **Input** | | |
| Source names | Water | |
| **General parameters** | | |
| Parameters | Value | |
| Temperature in (ºC) | 25 | |
| Temperature out (ºC) | 55 | |
| **Cost related parameters** | | |
| Reference flow type | Entering mass flow | |
| Reference flow (t/h) | 0.63 | |
| Components | Solids of the input streams | |
| Reference cost (M€) | 9 | |
| Reference Year | 2006 | |
| Exponent | 0.33 | |
| **Utility requirements – Electricity requirements** | | |
| Reference flow type | Entering mass flow | |
| Energy consumption (MWh/t) | 0.01 | |
| Components | Solids of the input streams | |
| **Heating Requirements** | | |
| Reference flow type | Entering Flow Heat Capacity | |
| Required Cooling / Heating (∆T) | 30 | |
| Components | Liquids of the input streams | |
| **Mixing Coefficients** | | |
| Mixing coefficient | 0.10 | |
| Mixing Table: Reference flow 1 | Reference Flow Type | Entering mass flow |
| Components | All components of the BSG |
| Mixing Table: Reference flow 2 | Reference Flow Type | Entering mass flow |
| Components | H2O |
| **Reactions** | | |
| Reaction name | Conversion (%) | Reactant |
| Acetyl groups DA | 100 | Acetyl groups |
| Cellulose DA | 100 | Cellulose |
| Hemicellulose DA | 100 | Hemicellulose |
| Lipids DA | 100 | Lipids |
| Proteins DA | 100 | Proteins |
| Starch DA | 100 | Starch |
| **Separation efficiency** | | |
| Separation information | A first flow with CH4 and CO2 | |
| A second flow with the solids and a 20% of liquid | |

Table 23. Definition of the composting unit for compost production

|  |  |  |
| --- | --- | --- |
| **Composting** | | |
| **General parameters** | | |
| Parameters | Value | |
| Temperature in (ºC) | 55 | |
| Temperature out (ºC) | 80 | |
| **Cost related parameters** | | |
| Reference flow type | Entering mass flow | |
| Reference flow (t/h) | 3.75 | |
| Components | Solids of the input streams | |
| Reference cost (M€) | 0.48 | |
| Reference Year | 2006 | |
| Exponent | 0.60 | |
| **Utility requirements – Electricity requirements** | | |
| Reference flow type | Entering mass flow | |
| Energy consumption (MWh/t) | 0.035 | |
| Components | Solids of the input streams | |
| **Reactions** | | |
| Product | Yield factor | Inert Chemicals |
| Compost | 0.715 | H2O |
| **Separation efficiency** | | |
| Separation information | Compost with a 5% humidity as final product | |

Table 24. Definition of the CHP unit for heat and power production (Part 1)

|  |  |  |
| --- | --- | --- |
| **CHP** | | |
| **Inputs** | | |
| Source name | Air | |
| **General parameters** | | |
| Parameters | Value | |
| Temperature in (ºC) | 55 | |
| Temperature out (ºC) | 90 | |
| **Energy efficiency** | | |
| Energy Type | Combined Heat and Power | |
| Conversion Efficiency | Efficiency | 0.35 |
| Heat efficiency | 0.50 |
| **Cost related parameters** | | |
| Reference flow type | Entering mass flow | |
| Reference flow (t/h) | 5 | |
| Components | CH4 | |
| Reference cost (M€) | 0.001 | |
| Reference Year | 2021 | |
| Exponent | 1 | |

Table 24. Definition of the CHP unit for heat and power production (Part 2)

|  |  |  |
| --- | --- | --- |
| **CHP** | | |
| **Utility requirements – Electricity requirements** | | |
| Reference flow type | Entering mass flow | |
| Energy consumption (MWh/t) | 0.24 | |
| Components | O2; N2 | |
| **Reactions** | | |
| Reaction name | Conversion | Reactant |
| CHP | 100 | CH4 |
| **Mixing Coefficients** | | |
| Mixing coefficient | 6.51 | |
| Mixing Table: Reference flow 1 | Reference Flow Type | Entering mass flow |
| Components | O2; N2 |
| Mixing Table: Reference flow 2 | Reference Flow Type | Entering mass flow |
| Components | CH4; CO2 |
| **Separation efficiency** | | |
| Separation information | It is not necessary to define compound separation in this unit, although a warning message appears when completing the tabs | |

Table 25. Definition of the bioupgrade unit for biogas production

|  |  |
| --- | --- |
| **Bioupgrade** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 55 |
| Temperature out (ºC) | 55 |
| **Cost related parameters** | |
| Reference flow type | Entering mass flow |
| Reference flow (t/h) | 3.22 |
| Components | CH4; CO2 |
| Reference cost (M€) | 1.94 |
| Reference Year | 2006 |
| Exponent | 0.93 |
| **Utility requirements – Electricity requirements** | |
| Reference flow type | Entering mass flow |
| Energy consumption (MWh/t) | 0.2633 |
| Components | CH4; CO2 |
| **Separation efficiency** | |
| Separation information | CH4 97.5% of mass purity as final product |

# Explore superstructure’s mapping

Feel free to connect routes to reduce waste, explore possibilities of combining routes to produce multiple products, or modify/add inputs and units to the superstructure based on prior knowledge. Trying diverse types of simple optimization or calculating the impacts of LCA to perform multi-objective optimization is algo encouraged.