# 1 Introduction

Tomato pomace is the main by-product of tomato processing industries with an estimated annual generation of around 330,000 tons in Europe in 2021. This residue, consisting primarily of peels, seeds and residual pulp, typically represents the 5-10% of the total weight of processed tomatoes.

The chemical composition of tomato pomace depends on the ratio of peels and seeds. In this matter, the tomato seeds represent the main source of protein and fats, while the peels are rich in cutin, a natural polymer, and provide phenolic compounds such as lycopene.

Tomato pomace is currently used for animal feed, composting or landfilling. However, its heterogeneous and composition makes it an attractive feedstock for the development of biorefineries. In this regard, the present case study explores alternative valorisation paths for tomato pomace based on extraction technologies.

# 2 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 half of the approximate amount of tomato pomace processed by Tomapaint company.

Table 1. Definition of general system parameters

|  |  |  |
| --- | --- | --- |
|  | **Parameter** | **Value** |
| **Specific production** | Load type | Substrate |
| Main product / Substrate | Tomato Pomace |
| Substrate load (t/y) | 1665 |
| **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 |

# 3 Define the chemical compounds

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

Table 2. Compounds required for the production systems proposed

|  |  |  |
| --- | --- | --- |
| **Component** | **Heat capacity (kJ/kg·K)** | **Molecular weight (g/mol)** |
| Tomato pomace | 1.36 | - |
| Tomato peels | 1.36 | - |
| Tomato seeds | 1.36 | ­- |
| H2O | 4.18 | 18.01 |
| NaOH | 1.40 | 40.00 |
| TRIS | - | 121.14 |
| EtOH | 2.44 | 46.07 |
| Cholinium Hexanoate | 2.05 | 236.00 |
| Lactic Acid | 2.43 | 90.08 |
| Choline Chloride | 1.78 | 139.62 |
| Ash | - | - |
| Protein | 1.36 | - |
| Fats | 1.36 | - |
| Cellulose | 1.36 | - |
| Hemicellulose | 1.36 | - |
| Starch | 1.26 | - |
| Sugars | 1.50 | - |
| Phenolics | - | - |
| Peptides | 1.36 | - |
| Cutin | 1.20 | - |
| Trypsin | - | - |
| Free lycopene | - | - |
| Free cutin | - | - |

# 4 Define the reactions

Table 3 specify the mass stoichiometry of all the reactions considered in the superstructure.

Table 3. Reactions (mass stoichiometry)

|  |  |
| --- | --- |
| **Reaction name** | **Reaction equation** |
| Peels\_Seeds\_sep | 1 Tomato pomace 🡪 0.27 Tomato peels + 0.33 Tomato seeds + 0.40 Water |
| Seeds\_Grinding | 1 Seeds 🡪 0.30 Protein + 0.18 Cellulose + 0.17 Hemicellulose + 0.32 Fats + 0.03 Ash |
| Peels\_Grinding | 1 Peels 🡪 0.12 Protein + 0.18 Cellulose + 0.06 Hemicellulose + 0.26 Cutin + 0.08 Starch + 0.03 Phenolics + 0.22 Sugars + 0.05 Ash |
| Peptide\_Extraction | 1 Protein 🡪 1 Peptides |
| Lycopene\_Extraction | 1 Phenolics 🡪 1 Free Lycopene |
| Cutin\_Extraction | 1 Cutin 🡪 1 Free Cutin |

# 5 Define the utilities

Table 4 shows the costs and CO2 emissions associated with the electricity or heat exchange utilities used in the processes, including the typical temperature ranges.

Table 4. 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 |

# 6 Inputs information for superstructure mapping

Table 5, Table 6, Table 7, Table 8, Table 9 and Table 10 contain the information to define the inputs of the whole superstructure:

Table 5. Information to define Tomato Pomace input

|  |  |  |
| --- | --- | --- |
| **Source name** | Tomato pomace | |
| **Cost input (€/t)** | -22 | |
| **Components** | **Component name** | **Composition fraction** |
| Tomato pomace | 1.00 |

Table 6. Information to define Trypsin input

|  |  |  |
| --- | --- | --- |
| **Source name** | Trypsin | |
| **Cost input (€/t)** | 446 | |
| **Components** | **Component name** | **Composition fraction** |
| Water | 0.99 |
| Trypsin | 0.0099 |
| NaOH | 0.0001 |

Table 7. Information to define NADES input

|  |  |  |
| --- | --- | --- |
| **Source name** | NADES | |
| **Cost input (€/t)** | 5950 | |
| **Components** | **Component name** | **Composition fraction** |
| Water | 0.09 |
| Choline Chloride | 0.40 |
| Lactic Acid | 0.51 |

Table 8. Information to define Cholinium Hexanoate (IL) input

|  |  |  |
| --- | --- | --- |
| **Source name** | Cholinium Hexanoate | |
| **Cost input (€/t)** | 6240 | |
| **Components** | **Component name** | **Composition fraction** |
| Cholinium hexanoate | 1.00 |

Table 9. Information to define Ethanol solution input

|  |  |  |
| --- | --- | --- |
| **Source name** | Ethanol | |
| **Cost input (€/t)** | 532 | |
| **Components** | **Component name** | **Composition fraction** |
| Water | 0.20 |
| Ethanol | 0.80 |

Table 10. Information to define Water input

|  |  |  |
| --- | --- | --- |
| **Source name** | Water | |
| **Cost input (€/t)** | 1.9 | |
| **Components** | **Component name** | **Composition fraction** |
| Water | 1.00 |

# 7 Outputs information for superstructure mapping

Table 11 shows the main products obtained in the proposed production routes.

Table 11. Information to define the main products of the process

|  |  |  |
| --- | --- | --- |
| **Product name** | **Price output Input (€/t)** | **Product Type** |
| Lycopene pomade | 2930 | Main product |
| Peptide powder | 5500 | Main product |
| Cutin (polymer) | 3225 | Main product |

# 8 Pretreatment unit operations for the routes

Table 12, Table 13 and Table 15 provide the data required to represent the flotation, grinding of seeds and grinding of peels.

Table 12. Definition of the flotation unit (Part 1)

|  |  |
| --- | --- |
| **Flotation** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 25 |

Table 12. Definition of the flotation unit (Part 2)

|  |  |  |
| --- | --- | --- |
| **Flotation** | | |
| **Cost related parameters** | | |
| Reference flow type | Entering mass flow | |
| Reference flow (t/h) | 0.9 | |
| Components | Tomato pomace and water | |
| Reference cost (M€) | 0.15 | |
| Reference Year | 2020 | |
| Exponent | 0.67 | |
| **Utility requirements – Electricity requirements** | | |
| Reference flow type | Entering mass flow | |
| Energy consumption (MWh/t) | 0.3125 | |
| Components | Tomato pomace and water | |
| **Mixing Coefficients** | | |
| Mixing coefficient | 0.48 | |
| Mixing Table: Reference flow 1 | Reference Flow Type | Entering mass flow  Tomato pomace |
| Components |
| Mixing Table: Reference flow 2 | Reference Flow Type | Entering mass flow  Water |
| Components |
| **Reactions** | | |
| Reaction name | Conversion (%) | Reactant |
| Peels\_seeds\_sep | 100 | Tomato pomace |
| **Separation efficiency** | | |
| Separation information | Peels and seeds are separated  Water fraction for each stream is 0.001 | |

Table 13. Definition of the grinder for tomato seeds (Part 1)

|  |  |
| --- | --- |
| **Grinding I** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 25 |
| Table 14. **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 stream |

Table 14. Definition of the grinder for tomato seeds (Part 1)

|  |  |  |
| --- | --- | --- |
| **Grinding I** | | |
| **Reactions** | | |
| Reaction name | Conversion (%) | Reactant |
| Seeds\_Grinding | 100 | Tomato seeds |
| **Separation efficiency** | | |
| Separation information | All components enter the next unit | |

Table 15. Definition of the grinder for tomato peels

|  |  |  |
| --- | --- | --- |
| **Grinding II** | | |
| **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 stream | |
| 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 | |
| **Reactions** | | |
| Reaction name | Conversion (%) | Reactant |
| Peels\_Grinding | 100 | Tomato peels |
| **Separation efficiency** | | |
| Separation information | All components enter the next unit | |

# Route 1: Tomato seeds to protein powder

Table 16, Table 17, Table 19 and Table 20 provide the data required to represent the peptide extraction, separation of peptides from the tomato seeds and the removal of water by evaporation and drying.

Table 16. Definition of the peptide extraction unit (Part 1)

|  |  |
| --- | --- |
| **Enzymatic Treatment** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 37 |

Table 15. Definition of the peptide extraction unit (Part 2)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Enzymatic Treatment** | | | | |
| **Cost related parameters** | | | | |
| Reference flow type | | Entering mass flow | | |
| Reference flow (t/h) | | 0.8185 | | |
| Components | | All components of the input streams | | |
| Reference cost (M€) | | 0.04556 | | |
| Reference Year | | 2020 | | |
| Exponent | | 0.53 | | |
| **Utility requirements – Electricity requirements** | | | | |
| Reference flow type | Entering mass flow | | | |
| Energy consumption (MWh/t) | 0.00044 | | | |
| Components | All components of the input streams | | | |
| **Heating Requirements** | | | | |
| Reference flow type | Entering Flow Heat Capacity | | | |
| Required Cooling / Heating (∆T) | 12 | | | |
| Components | Water | | | |
| **Mixing Coefficients** | | | | |
| Mixing coefficient | | 0.17 | | |
| Mixing Table: Reference flow 1 | | Reference Flow Type | Entering mass flow | |
| Components | Trypsin | |
| Mixing Table: Reference flow 2 | | Reference Flow Type | Entering mass flow | |
| Components | Protein | |
| **Reactions** | | | | |
| Reaction name | Conversion (%) | | | Reactant |
| Peptide\_extraction | 12 | | | Protein |
| **Separation efficiency** | | | | |
| Separation information | All components enter the next unit | | | |

Table 17. Definition of the centrifuge (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 | All inputs |
| Reference cost (M€) | 0.213 |
| Reference Year | 2020 |
| Exponent | 0.38 |
| **Utility requirements – Electricity requirements** | |
| Reference flow type | Entering mass flow |
| Energy consumption (MWh/t) | 0.01 |
| Components | Solids of the input stream |

Table 18. Definition of the centrifuge (Part 2)

|  |  |
| --- | --- |
| **Centrifugation** | |
| **Separation efficiency** | |
| Separation information | Liquid stream with the main product |
| Solid stream with 15% liquid loss |

Table 19. Definition of the evaporator unit

|  |  |
| --- | --- |
| **Evaporation** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 100 |
| **Cost related parameters** | |
| Reference flow type | Entering Mass Flow |
| Reference flow (t/h) | 6761.78 |
| Components | All inputs |
| Reference cost (M€) | 0.729 |
| Reference Year | 2020 |
| Exponent | 0.5 |
| **Heating Requirements** | |
| Reference flow type | Entering Flow Heat Capacity |
| Required Cooling / Heating (∆T) | 75 |
| Components | Water |
| **Separation efficiency** | |
| Separation information | Peptides with 2% of water |

Table 20. Definition of the dryer

|  |  |
| --- | --- |
| **Drying** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 70 |
| Temperature out (ºC) | 100 |
| **Cost related parameters** | |
| Reference flow type | Entering Mass Flow |
| Reference flow (t/h) | 431.83 |
| Components | All inputs |
| Reference cost (M€) | 0.12758 |
| Reference Year | 2020 |
| Exponent | 0.52 |
| **Heating Requirements** | |
| Reference flow type | Entering Flow Heat Capacity |
| Required Cooling / Heating (∆T) | 75 |
| Components | Water |
| **Separation efficiency** | |
| Separation information | Peptides with 2% of water |

# Route 2: Tomato peels to phenolic extract

Table 21 provide the data to represent the solid liquid extraction of phenolic compounds from tomato peels.

Table 21. Definition of the Solid-Liquid extraction unit

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Solid-Liquid Extraction** | | | | |
| **General parameters** | | | | |
| Parameters | | Value | | |
| Temperature in (ºC) | | 25 | | |
| Temperature out (ºC) | | 65 | | |
| **Cost related parameters** | | | | |
| Reference flow type | | Entering mass flow | | |
| Reference flow (t/h) | | 6.67 | | |
| Components | | All components of the input streams | | |
| Reference cost (M€) | | 0.25856 | | |
| Reference Year | | 2020 | | |
| Exponent | | 0.4064 | | |
| **Utility requirements – Electricity requirements** | | | | |
| Reference flow type | Entering mass flow | | | |
| Energy consumption (MWh/t) | 0.01033 | | | |
| Components | All components of the input streams | | | |
| **Heating Requirements** | | | | |
| Reference flow type | Entering Flow Heat Capacity | | | |
| Required Cooling / Heating (∆T) | 40 | | | |
| Components | Water, lactic acid and choline chloride | | | |
| **Mixing Coefficients** | | | | |
| Mixing coefficient | | 18.73 | | |
| Mixing Table: Reference flow 1 | | Reference Flow Type | Entering mass flow | |
| Components | Water, lactic acid and choline chloride | |
| Mixing Table: Reference flow 2 | | Reference Flow Type | Entering mass flow | |
| Components | Grounded tomato peels | |
| **Reactions** | | | | |
| Reaction name | Conversion (%) | | | Reactant |
| Lycopene\_Extraction | 75 | | | Phenolics |
| **Separation efficiency** | | | | |
| Separation information | Extract: 75% of fats and phenolics  Raffinate: All the solids with 2% of NADES | | | |

# Route 3: Tomato peels to cutin

Table 22, Table 23, Table 24, Table 25 and Table 26 provide the data required to represent the solid liquid extraction of cutin, the pressure filtration using ethanol as washing agent, the recovery of both ethanol and ionic liquid via flash evaporation, the rotatory vacuum filtration to remove residual ethanol from the cutin and the final drying step for cutin.

Table 22. Definition of the solid-liquid extraction of cutin

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Solid-Liquid Extraction** | | | | |
| **General parameters** | | | | |
| Parameters | | Value | | |
| Temperature in (ºC) | | 25 | | |
| Temperature out (ºC) | | 100 | | |
| **Cost related parameters** | | | | |
| Reference flow type | | Entering mass flow | | |
| Reference flow (t/h) | | 0.8185 | | |
| Components | | All components of the input streams | | |
| Reference cost (M€) | | 0.04556 | | |
| Reference Year | | 2020 | | |
| Exponent | | 0.53 | | |
| **Utility requirements – Electricity requirements** | | | | |
| Reference flow type | Entering mass flow | | | |
| Energy consumption (MWh/t) | 0.00044 | | | |
| Components | All components of the input streams | | | |
| **Heating Requirements** | | | | |
| Reference flow type | Entering Flow Heat Capacity | | | |
| Required Cooling / Heating (∆T) | 75 | | | |
| Components | Solvent and water | | | |
| **Mixing Coefficients** | | | | |
| Mixing coefficient | | 10.0 | | |
| Mixing Table: Reference flow 1 | | Reference Flow Type | Entering mass flow | |
| Components | Cholinium Hexanoate | |
| Mixing Table: Reference flow 2 | | Reference Flow Type | Entering mass flow | |
| Components | Grounded tomato peels | |
| **Reactions** | | | | |
| Reaction name | Conversion (%) | | | Reactant |
| Cutin\_Extraction | 100 | | | Cutin |
| **Separation efficiency** | | | | |
| Separation information | All components to next unit | | | |

Table 23. Definition of the microfiltration (Part 1)

|  |  |
| --- | --- |
| **Micro-filtration** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 100 |
| Temperature out (ºC) | 70 |
| **Cost related parameters** | |
| Reference flow type | Entering Mass Flow |
| Reference flow (t/h) | 1.0 |
| Components | All from previous unit |
| Reference cost (M€) | 0.1455 |
| Reference Year | 2006 |
| Exponent | 0.92 |

Table 21. Definition of the microfiltration (Part 2)

|  |  |  |
| --- | --- | --- |
| **Micro-filtration** | | |
| **Annualized Capital Costs** | | |
| Turn Over Time (years) | 10.0 | |
| Turn Over Factor | 0.28 | |
| **Mixing Coefficients** | | |
| Mixing coefficient | 64 | |
| Mixing Table: Reference flow 1 | Reference Flow Type | Entering mass flow |
| Components | Ethanol |
| Mixing Table: Reference flow 2 | Reference Flow Type | Entering mass flow |
| Components | All solids |
| Components | Solids of the input streams | |
| **Separation efficiency** | | |
| Separation information | Cutin with 5% of ethanol and water | |

Table 24. Definition of the Flash unit

|  |  |  |
| --- | --- | --- |
| **Flash** | | |
| **General parameters** | | |
| Parameters | Value | |
| Temperature in (ºC) | 25 | |
| Temperature out (ºC) | 82 | |
| **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) | 57 | |
| Components | Liquids of the input streams | |
| **Separation efficiency** | | |
| Separation information | | 85% of ethanol recovered |

Table 25. Definition of the rotatory filter (Part 1)

|  |  |
| --- | --- |
| **Rotatory filter** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 25 |
| **Utility requirements – Electricity requirements** | |
| Reference flow type | Entering Mass Flow |
| Energy consumption (MWh/t) | 0.0055 |

Table 23. Definition of the rotatory filter (Part 2)

|  |  |  |
| --- | --- | --- |
| **Rotatory filter** | | |
| **Cost related parameters** | | |
| Reference flow type | Entering Mass Flow | |
| Reference flow (t/h) | 5.0 | |
| Components | Cutin, ethanol and water | |
| Reference cost (M€) | 0.036 | |
| Reference Year | 2006 | |
| Exponent | 0.53 | |
| **Mixing Coefficients** | | |
| Mixing coefficient | 0.0024 | |
| Mixing Table: Reference flow 1 | Reference Flow Type | Entering mass flow |
| Components | Free Cutin |
| Mixing Table: Reference flow 2 | Reference Flow Type | Entering mass flow |
| Components | Water |
| Components | Solids of the input streams | |
| **Separation efficiency** | | |
| Separation information | Cutin with 1% of water | |

Table 26. Definition of the dryer

|  |  |
| --- | --- |
| **Drying** | |
| **General parameters** | |
| Parameters | Value |
| Temperature in (ºC) | 25 |
| Temperature out (ºC) | 100 |
| **Cost related parameters** | |
| Reference flow type | Entering Mass Flow |
| Reference flow (t/h) | 431.83 |
| Components | All inputs |
| Reference cost (M€) | 0.12758 |
| Reference Year | 2020 |
| Exponent | 0.52 |
| **Heating Requirements** | |
| Reference flow type | Entering Flow Heat Capacity |
| Required Cooling / Heating (∆T) | 75 |
| Components | Water |
| **Separation efficiency** | |
| Separation information | Cutin with 2% of water |

# 12 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 training. Trying diverse types of simple optimization or calculating the impacts of LCA to perform multi-objective optimization is algo encouraged.