**SUPPLEMENTARY MATERIAL**

**Table Captions**

Table S1. Input and output data for process of biodiesel production.

**Table S2.** Input and output data for alcohol recycle unit.

**Table S3.** Input and output data for etherification reaction using ethanol and isopropanol at 110ºC and molar ratio of 1:6 (glycerol/alcohol).

**Table S4.** Input and output data from DWSIM for etherification reaction using ethanol and isopropanol at 110ºC and molar ratio of 1:12 (glycerol/alcohol).

Table S5. Input and output data for ether purification process (etherification using glycerol/ethanol molar ratio of 1:3 at 110ºC).

Table S6. Input and output data for ether purification process (etherification using glycerol/isopropanol molar ratio of 1:3 at 110ºC).

**Table S1**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Conditions** | **Input** |  | **Output** | |
| STR-01 |  | Biodiesel | Crude glycerol |
| **Temperature (ºC)** | 28.7 |  | 60.0 | 60.0 |
| **Pressure (bar)** | 1.01 |  | 1.01 | 1.01 |
| **Mass Flow (kg/h)** | 1227.12 |  | 1004.31 | 222.81 |
| **Volumetric Flow (m3/h)** | 1.347 |  | 1.178 | 0.260 |
| **Specific Enthalpy (kJ/kg)** | -203.64 |  | -232.52 | -936.48 |
| **Component mole fraction** |  |  |  |  |
| **Triolein** | 0.138 |  | 0.000 | 0.017 |
| **Methanol** | 0.830 |  | 0.436 | 0.728 |
| **Sodium Hydroxide** | 0.030 |  | 0.030 | 0.051 |
| **Biodiesel** | 0.000 |  | 0.394 | 0.000 |
| **Crude glycerol** | 0.000 |  | 0.131 | 0.219 |

STR-01: Mixture of vegetable oil, methanol and sodium hydroxide.

Table S2

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Alcohol recovery / Ethanol** | | | | | | | |
| **Conditions** | **Input** | |  | **Output** | | | |
| Polar comp. | |  | STR-67 | | Alcohol | |
| **Temperature (ºC)** | 79.9 | |  | -10.0 | | -10.0 | |
| **Pressure (bar)** | 1.01 | |  | 1.01 | | 1.01 | |
| **Mass Flow (kg/h)** | 117.89 | |  | 51.00 | | 66.89 | |
| **Volumetric Flow (m3/h)** | 0.137 | |  | 0.050 | | 0.082 | |
| **Spec. Enthalpy (kJ/kg)** | -1162.72 | |  | -1931.98 | | -1012.28 | |
| **Component mole fraction** | | | | | | | |
| **Ethanol** | 0.434 | |  | 0.000 | | 1.000 | |
| **Glycerol** | 0.068 | |  | 0.121 | | 0.000 | |
| **Water** | 0.496 | |  | 0.878 | | 0.000 | |
| **Alcohol recovery / Isopropanol** | | | | | | | |
| **Conditions** | | **Input** |  | | **Output** | | | |
| Polar comp. |  | | STR-67 | | Alcohol | |
| **Temperature (ºC)** | | 85.8 |  | | -10.0 | | -10.0 | |
| **Pressure (bar)** | | 1.01 |  | | 1.01 | | 1.01 | |
| **Mass Flow (kg/h)** | | 203.86 |  | | 52.78 | | 151.07 | |
| **Volumetric Flow (m3/h)** | | 26.267 |  | | 0.043 | | 0.186 | |
| **Spec. Enthalpy (kJ/kg)** | | -527.98 |  | | -1523.60 | | -844.97 | |
| **Component mole fraction** | | | | | | | |
| **Isopropanol** | | 0.704 |  | | 0.000 | | 1.000 | |
| **Glycerol** | | 0.127 |  | | 0.433 | | 0.000 | |
| **Water** | | 0.167 |  | | 0.566 | | 0.000 | |

STR-67: Mixture of water and glycerol.

Table S3

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Etherification with ethanol (1:6 molar ratio)** | | | | | | | | |
| **Conditions** | **Input** | | | |  | **Output** | | |
| **Glycerol** | | **Ethanol** | |  | **STR-12** | **STR-13** | |
| **Temperature (ºC)** | 229.2 | | 25.0 | |  | 110.0 | 110.0 | |
| **Pressure (bar)** | 1.01 | | 1.01 | |  | 1.01 | 1.01 | |
| **Mass Flow (kg/h)** | 95.51 | | 286.66 | |  | 219.59 | 162.57 | |
| **Volumetric Flow (m3/h)** | 0.087 | | 0.364 | |  | 166.250 | 0.188 | |
| **Spec. Enthalpy (kJ/kg)** | -475.76 | | -922.64 | |  | 134.65 | -587.50 | |
| **Component mole fraction** | | | | | | | | |
| **Ethanol** | 0.000 | | 1.000 | |  | 0.829 | 0.259 | |
| **Glycerol** | 1.000 | | 0.000 | |  | 0.000 | 0.112 | |
| **3-ethoxypropan-1,2-diol** | 0.000 | | 0.000 | |  | 0.000 | 0.154 | |
| **1,3-diethoxypropan-2-ol** | 0.000 | | 0.000 | |  | 0.002 | 0.255 | |
| **1,2,3-triethoxypropane** | 0.000 | | 0.000 | |  | 0.000 | 0.000 | |
| **Water** | 0.000 | | 0.000 | |  | 0.169 | 0.220 | |
| **Etherification with isopropanol (1:6 molar ratio)** | | | | | | | | |
| **Conditions** | | **Input** | |  | | **Output** | | |
| **Glycerol** | **Isopropanol** |  | | **STR-12** | | **STR-13** |
| **Temperature (ºC)** | | 229.2 | 25.0 |  | | 110.0 | | 110.0 |
| **Pressure (bar)** | | 1.01 | 1.01 |  | | 1.01 | | 1.01 |
| **Mass Flow (kg/h)** | | 95.51 | 373.94 |  | | 313.26 | | 156.19 |
| **Volumetric Flow (m3/h)** | | 0.087 | 0.478 |  | | 176.982 | | 0.174 |
| **Spec. Enthalpy (kJ/kg)** | | -475.76 | -754.44 |  | | 140.72 | | -615.86 |
| **Component mole fraction** | | | | | | | | |
| **Isopropanol** | | 0.000 | 1.000 |  | | 0.894 | | 0.309 |
| **Glycerol** | | 1.000 | 0.000 |  | | 0.000 | | 0.224 |
| **3-isopropoxypropan-1,2-diol** | | 0.000 | 0.000 |  | | 0.000 | | 0.402 |
| **1,3-di-isopropoxypropan-2-ol** | | 0.000 | 0.000 |  | | 0.000 | | 0.010 |
| **Water** | | 0.000 | 0.000 |  | | 0.106 | | 0.055 |

STR-12: Reaction mixture (Vapor phase); STR-13: Reaction mixture (Liquid phase).

Table S4

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Etherification with ethanol (1:12 molar ratio)** | | | | | | | | |
| **Conditions** | **Input** | | | |  | **Output** | | |
| **Glycerol** | | **Ethanol** | |  | **STR-12** | **STR-13** | |
| **Temperature (ºC)** | 229.2 | | 25.0 | |  | 110.0 | 110.0 | |
| **Pressure (bar)** | 1.01 | | 1.01 | |  | 1.01 | 1.01 | |
| **Mass Flow (kg/h)** | 95.51 | | 573.32 | |  | 495.01 | 173.82 | |
| **Volumetric Flow (m3/h)** | 0.087 | | 0.729 | |  | 365.001 | 0.196 | |
| **Spec. Enthalpy (kJ/kg)** | -475.76 | | -922.64 | |  | 134.14 | -465.04 | |
| **Component mole fraction** | | | | | | | | |
| **Ethanol** | 0.000 | | 1.000 | |  | 0.860 | 0.281 | |
| **Glycerol** | 1.000 | | 0.000 | |  | 0.000 | 0.092 | |
| **3-ethoxypropan-1,2-diol** | 0.000 | | 0.000 | |  | 0.000 | 0.089 | |
| **1,3-diethoxypropan-2-ol** | 0.000 | | 0.000 | |  | 0.001 | 0.167 | |
| **1,2,3-triethoxypropane** | 0.000 | | 0.000 | |  | 0.002 | 0.185 | |
| **Water** | 0.000 | | 0.000 | |  | 0.136 | 0.186 | |
| **Etherification with isopropanol (1:12 molar ratio)** | | | | | | | | |
| **Conditions** | | **Input** | |  | | **Output** | | |
| **Glycerol** | **Isopropanol** |  | | **STR-12** | | **STR-13** |
| **Temperature (ºC)** | | 229.2 | 25.0 |  | | 110.0 | | 110.0 |
| **Pressure (bar)** | | 1.01 | 1.01 |  | | 1.01 | | 1.01 |
| **Mass Flow (kg/h)** | | 95.51 | 745.35 |  | | 676.14 | | 164.72 |
| **Volumetric Flow (m3/h)** | | 0.087 | 0.953 |  | | 371.136 | | 0.188 |
| **Spec. Enthalpy (kJ/kg)** | | -475.76 | -754.44 |  | | 140.46 | | -588.77 |
| **Component mole fraction** | | | | | | | | |
| **Isopropanol** | | 0.000 | 1.000 |  | | 0.933 | | 0.335 |
| **Glycerol** | | 1.000 | 0.000 |  | | 0.000 | | 0.128 |
| **3-isopropoxypropan-1,2-diol** | | 0.000 | 0.000 |  | | 0.000 | | 0.494 |
| **1,3-di-isopropoxypropan-2-ol** | | 0.000 | 0.000 |  | | 0.000 | | 0.011 |
| **Water** | | 0.000 | 0.000 |  | | 0.067 | | 0.032 |

STR-12: Reaction mixture (Vapor phase); STR-13: Reaction mixture (Liquid phase).

Table S5

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Ether purification for simulation using ethanol (1:3 molar ratio)** | | | | | | | |
| **Conditions** | **Input** | | |  | **Output** | | |
| **STR-12** | **STR-13** | **Solvent** |  | **Ethers** | **Solvent** | **Polar Comp.** |
| **Temperature (ºC)** | 110.0 | 110.0 | 25.0 |  | 213.9 | 69.8 | 79.8 |
| **Pressure (bar)** | 1.01 | 1.01 | 1.01 |  | 1.01 | 1.01 | 1.01 |
| **Mass Flow (kg/h)** | 59.62 | 179.21 | 238.83 |  | 116.12 | 243.66 | 117.88 |
| **Molar Flow (kmol/h)** | 1.65 | 2.50 | 2.77 |  | 0.78 | 2.80 | 3.34 |
| **Vol. Flow (m3/h)** | 51.91 | 0.20 | 0.36 |  | 0.14 | 53.65 | 0.14 |
| **Spec. Enthalpy (kJ/kmol)** | 137.42 | -614.17 | -366.01 |  | -92.81 | -30.33 | -1173.78 |
| **Component mole fraction** | | | | | | | |
| **Ethanol** | 0.636 | 0.160 | 0.000 |  | 0.000 | 0.000 | 0.434 |
| **Glycerol** | 0.000 | 0.092 | 0.000 |  | 0.000 | 0.000 | 0.068 |
| **3-ethoxypropan-1,2-diol** | 0.000 | 0.095 | 0.000 |  | 0.304 | 0.000 | 0.000 |
| **1,3-dietoxipropan-2-ol** | 0.001 | 0.115 | 0.000 |  | 0.361 | 0.001 | 0.000 |
| **1,2,3-triethoxypropane** | 0.001 | 0.112 | 0.000 |  | 0.324 | 0.010 | 0.000 |
| **Water** | 0.361 | 0.425 | 0.000 |  | 0.000 | 0.000 | 0.496 |
| **N-hexane** | 0.000 | 0.000 | 1.000 |  | 0.010 | 0.988 | 0.000 |

STR-12: Reaction mixture (Vapor phase); STR-13: Reaction mixture (Liquid phase).

**Table S6**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Ether purification for simulation using isopropanol (1:3 molar ratio)** | | | | | | | |
| **Conditions** | **Input** | | |  | **Output** | | |
| **STR-12** | **STR-13** | **Hexane** |  | **Ethers** | **Hexane** | **Polar Comp.** |
| **Temperature (ºC)** | 110.00 | 110.00 | 25.00 |  | 224.30 | 69.09 | 81.93 |
| **Pressure (bar)** | 1.01 | 1.01 | 1.01 |  | 1.01 | 1.01 | 1.01 |
| **Mass Flow (kg/h)** | 675.91 | 164.72 | 840.63 |  | 97.85 | 854.59 | 728.83 |
| **Molar Flow (kmol/h)** | 11.80 | 1.63 | 9.75 |  | 0.73 | 9.85 | 12.61 |
| **Vol. Flow (m3/h)** | 371.02 | 0.19 | 1.28 |  | 0.12 | 1.38 | 0.98 |
| **Spec. Enthalpy (kJ/kmol)** | 140.44 | -587.04 | -366.01 |  | -277.79 | -261.67 | -615.80 |
| **Component mole fraction** | | | | | | | |
| **Isopropanol** | 0.932 | 0.335 | 0.000 |  | 0.000 | 0.000 | 0.916 |
| **Glycerol** | 0.000 | 0.127 | 0.000 |  | 0.000 | 0.000 | 0.016 |
| **3-ethoxypropan-1,2-diol** | 0.000 | 0.494 | 0.000 |  | 0.975 | 0.010 | 0.000 |
| **1,3-dietoxipropan-2-ol** | 0.000 | 0.011 | 0.000 |  | 0.014 | 0.001 | 0.000 |
| **Water** | 0.067 | 0.031 | 0.000 |  | 0.000 | 0.000 | 0.067 |
| **N-hexane** | 0.000 | 0.000 | 1.000 |  | 0.010 | 0.989 | 0.000 |

STR-12: Reaction mixture (Vapor phase); STR-13: Reaction mixture (Liquid phase).