Table S1: Pure glycerol Section 100 stream table.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-001** | **S-002** | **S-003** | **S-004** | **S-005** | **S-006** | **S-007** | **S-008** | **S-009** | **S-010** | **S-011** | **S-012** | **S-013** |
| **Mass Flowrate (MT/batch)** | 47.337 | 14.142 | 33.194 | 183.617 | 47.653 | 183.617 | 47.653 | 183.617 | 47.653 | 183.617 | 18.206 | 4.273 | 47.653 |
| **Temperature (οC)** | 50.3 | 50.3 | 50.3 | 26.4 | 40.4 | 26.4 | 40.4 | 37.0 | 37.0 | 37.0 | 25.0 | 25.0 | 40.4 |
| **Pressure (bar)** | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **(NH4)2HPO4** | 0.0000 | 0.0000 | 0.0000 | 637.206 | 128.197 | 637.206 | 128.1969 | 637.2061 | 128.1969 | 637.2061 | 637.2061 | 128.1969 | 128.1969 |
| **CaCl2** | 0.0000 | 0.0000 | 0.0000 | 2.0026 | 0.0000 | 2.0026 | 0.0000 | 2.0026 | 0.0000 | 2.0026 | 2.0026 | 0.0000 | 0.0000 |
| **CoCl2** | 0.0000 | 0.0000 | 0.0000 | 0.0364 | 0.0282 | 0.0364 | 0.0282 | 0.0364 | 0.0282 | 0.0364 | 0.0364 | 0.0282 | 0.0282 |
| **CuCl2** | 0.0000 | 0.0000 | 0.0000 | 0.0182 | 0.0141 | 0.0182 | 0.0141 | 0.0182 | 0.0141 | 0.0182 | 0.0182 | 0.0141 | 0.0141 |
| **FeCl3(aq)** | 0.0000 | 0.0000 | 0.0000 | 0.2915 | 0.2258 | 0.2915 | 0.2258 | 0.2915 | 0.2258 | 0.2915 | 0.2915 | 0.2258 | 0.2258 |
| **Glycerol** | 36562.91 | 10923.53 | 25639.37 | 10923.5 | 25639.4 | 10923.5 | 25639.37 | 10923.534 | 25639.372 | 10923.53 | 0.0000 | 0.0000 | 25639.3715 |
| **H3BO3** | 0.0000 | 0.0000 | 0.0000 | 0.0091 | 0.0071 | 0.0091 | 0.0071 | 0.0091 | 0.0071 | 0.0091 | 0.0091 | 0.0071 | 0.0071 |
| **HCl(aq)** | 0.0000 | 0.0000 | 0.0000 | 0.6643 | 0.5146 | 0.6643 | 0.5146 | 0.6643 | 0.5146 | 0.6643 | 0.6643 | 0.5146 | 0.5146 |
| **Impurities** | 48.7505 | 14.5647 | 34.1858 | 14.5647 | 34.1858 | 14.5647 | 34.1858 | 14.5647 | 34.1858 | 14.5647 | 0.0000 | 0.0000 | 34.1858 |
| **K2HPO4** | 0.0000 | 0.0000 | 0.0000 | 910.295 | 0.0000 | 910.295 | 0.0000 | 910.2945 | 0.0000 | 910.2945 | 910.2945 | 0.0000 | 0.0000 |
| **KH2PO4** | 0.0000 | 0.0000 | 0.0000 | 637.206 | 0.0000 | 637.206 | 0.0000 | 637.2061 | 0.0000 | 637.2061 | 637.2061 | 0.0000 | 0.0000 |
| **MgSO4(aq)** | 0.0000 | 0.0000 | 0.0000 | 21.6650 | 10.2557 | 21.6650 | 10.2557 | 21.6650 | 10.2557 | 21.6650 | 21.6650 | 10.2557 | 10.2557 |
| **MnCl2** | 0.0000 | 0.0000 | 0.0000 | 0.1002 | 0.0776 | 0.1002 | 0.0776 | 0.1002 | 0.0776 | 0.1002 | 0.1002 | 0.0776 | 0.0776 |
| **Water** | 10725.12 | 3204.237 | 7520.882 | 170467 | 21840.1 | 170470 | 21840.10 | 170469.71 | 21840.10 | 170470 | 15996.36 | 4133.88 | 21840.10 |

Table S2: Pure glycerol Section 200 stream table (1).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-015** | **S-016** | **S-017** | **S-018** | **S-019** | **S-020** | **S-021** | **S-022** | **S-023** | **S-024** | **S-025** | **S-026** | **S-027** | **S-028** | **S-029** |
| **Mass Flowrate (MT/batch)** | 0.095 | 0.014 | 57.106 | 0.006 | 135.263 | 135.263 | 135.263 | 0.031 | 0.113 | 0.033 | 1.429 | 0.006 | 0.422 | 1.513 | 0.457 |
| **Temperature (οC)** | 37.0 | 25.0 | 25.0 | 25.0 | 25.0 | 25.0 | 37.0 | 37.0 | 37.0 | 37.0 | 37.0 | 25.0 | 37.0 | 37.0 | 37.0 |
| **Pressure (bar)** | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 3.013 | 3.013 | 1.013 | 1.013 | 1.013 | 1.013 | 3.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **(NH4)2HPO4** | 0.3301 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.2282 | 0.0000 | 4.9575 | 0.0000 | 0.0000 | 3.6458 | 0.0000 |
| **Biomass** | 0.0000 | 0.1419 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 2.1789 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 32.9772 | 0.0000 |
| **CaCl2** | 0.0010 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0010 | 0.0000 | 0.0156 | 0.0000 | 0.0000 | 0.0166 | 0.0000 |
| **CoCl2** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0003 | 0.0000 | 0.0000 | 0.0003 | 0.0000 |
| **FeCl3(aq)** | 0.0002 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0002 | 0.0000 | 0.0023 | 0.0000 | 0.0000 | 0.0024 | 0.0000 |
| **Glycerol** | 5.6584 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.5658 | 0.0000 | 84.9851 | 0.0000 | 0.0000 | 8.5551 | 0.0000 |
| **HCl(aq)** | 0.0003 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0003 | 0.0000 | 0.0052 | 0.0000 | 0.0000 | 0.0055 | 0.0000 |
| **Impurities** | 0.0075 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0075 | 0.0000 | 0.1133 | 0.0000 | 0.0000 | 0.1209 | 0.0000 |
| **K2CO3** | 0.0000 | 0.0000 | 22842.68 | 2.2697 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 2.2697 | 0.0000 | 0.0000 | 2.2697 | 0.0000 | 4.5395 | 0.0000 |
| **K2HPO4** | 0.4715 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.4206 | 0.0000 | 7.0821 | 0.0000 | 0.0000 | 6.7327 | 0.0000 |
| **KH2PO4** | 0.3301 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.2791 | 0.0000 | 4.9575 | 0.0000 | 0.0000 | 4.4667 | 0.0000 |
| **Nitrogen** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 103763 | 103763 | 103763 | 23.3932 | 0.0000 | 23.4959 | 0.0000 | 0.0000 | 323.3923 | 0.0000 | 324.7842 |
| **Oxygen** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 31500.4 | 31500.4 | 31500.42 | 7.1017 | 0.0000 | 2.2491 | 0.0000 | 0.0000 | 98.1756 | 0.0000 | 24.7605 |
| **Water** | 88.3033 | 14.0440 | 34264.02 | 3.4046 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 106.7704 | 0.0000 | 1326.2543 | 3.4046 | 0.0000 | 1451.8285 | 0.0000 |

Table S3: Pure glycerol Section 200 stream table (2).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-030** | **S-031** | **S-032** | **S-033** | **S-034** | **S-035** | **S-036** | **S-037** | **S-038** | **S-039** | **S-040** | **S-041** | **S-042** | **S-043** |
| **Mass Flowrate (MT/batch)** | 21.127 | 0.006 | 6.188 | 22.144 | 6.715 | 160.967 | 0.006 | 57.084 | 50.078 | 47.653 | 78.546 | 276.749 | 140.051 | 276.749 |
| **Temperature (οC)** | 37.0 | 25.0 | 37.0 | 37.0 | 37.0 | 37.0 | 25.0 | 25.0 | 37.0 | 37.0 | 37.0 | 39.0 | 39.0 | 39.0 |
| **Pressure (bar)** | 1.013 | 1.013 | 3.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 3.013 | 1.013 | 3.013 | 1.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **(NH4)2HPO4** | 73.3163 | 0.0000 | 0.0000 | 54.1848 | 0.0000 | 558.6023 | 0.0000 | 0.0000 | 0.0000 | 128.1969 | 0.0000 | 566.3375 | 0.0000 | 566.3375 |
| **Biomass** | 0.0000 | 0.0000 | 0.0000 | 488.523 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 3981.4521 | 0.0000 | 3981.4521 |
| **CO2** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 1592.70 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 19483.8913 | 0.0000 |
| **FeCl3(aq)** | 0.0335 | 0.0000 | 0.0000 | 0.0360 | 0.0000 | 0.2556 | 0.0000 | 0.0000 | 0.0000 | 0.2258 | 0.0000 | 0.5173 | 0.0000 | 0.5173 |
| **Glycerol** | 1256.851 | 0.0000 | 0.0000 | 126.541 | 0.0000 | 9576.04 | 0.0000 | 0.0000 | 0.0000 | 25639.37 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| **Impurities** | 1.6758 | 0.0000 | 0.0000 | 1.7967 | 0.0000 | 12.7681 | 0.0000 | 0.0000 | 0.0000 | 34.1858 | 0.0000 | 541.5215 | 0.0000 | 541.5215 |
| **Acetate Salt** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 1288.6075 | 0.0000 | 1288.6075 |
| **Succinate Salt** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 30807.153 | 0.0000 | 30807.1531 |
| **K2CO3** | 0.0000 | 2.2697 | 0.0000 | 6.8092 | 0.0000 | 0.0000 | 2.2697 | 22833.600 | 0.0000 | 0.0000 | 0.0000 | 23.1900 | 0.0000 | 23.1900 |
| **K2HPO4** | 104.7376 | 0.0000 | 0.0000 | 100.082 | 0.0000 | 798.003 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 810.7617 | 0.0000 | 810.7617 |
| **KH2PO4** | 73.3163 | 0.0000 | 0.0000 | 66.3943 | 0.0000 | 558.602 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 537.6734 | 0.0000 | 537.6734 |
| **MgSO4(aq)** | 2.4928 | 0.0000 | 0.0000 | 2.6725 | 0.0000 | 18.9925 | 0.0000 | 0.0000 | 0.0000 | 10.2557 | 0.0000 | 31.9208 | 0.0000 | 31.9208 |
| **N2** | 0.0000 | 0.0000 | 4746.958 | 0.0000 | 4767.36 | 0.0000 | 0.0000 | 0.0000 | 38415.544 | 0.0000 | 60253.6595 | 0.0000 | 98919.8092 | 0.0000 |
| **O2** | 0.0000 | 0.0000 | 1441.085 | 0.0000 | 355.140 | 0.0000 | 0.0000 | 0.0000 | 11662.215 | 0.0000 | 18291.8436 | 0.0000 | 21647.1353 | 0.0000 |
| **Water** | 19614.07 | 3.4046 | 0.0000 | 21297.1 | 0.0000 | 149441 | 3.4046 | 34250.400 | 0.0000 | 21840.10 | 0.0000 | 238156.27 | 0.0000 | 238156.274 |

Table S4: Pure glycerol Section 300(a) stream table (1).

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-044** | **S-045** | **S-046** | **S-047** | **S-048** | **S-049** | **S-050** | **S-051** | **S-052** |
| **Mass Flowrate (MT/batch)** | 248.306 | 28.442 | 248.040 | 0.2673 | 248.037 | 248.037 | 248.037 | 836.010 | 97.358 |
| **Temperature (οC)** | 39.8 | 39.8 | 40.1 | 40.1 | 39.7 | 39.7 | 52.0 | 25.0 | 25.0 |
| **Pressure (bar)** | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **(NH4)2HPO4** | 547.0792 | 19.2583 | 546.9287 | 0.1504 | 546.929 | 546.929 | 546.9287 | 0.0000 | 0.0000 |
| **Acetic Anion** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 748.734 | 748.734 | 748.7344 | 0.0000 | 0.0000 |
| **Biomass** | 39.8145 | 3941.638 | 0.0000 | 39.8145 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| **CaCl2** | 1.9345 | 0.0681 | 1.9340 | 0.0005 | 1.9340 | 1.9340 | 1.9345 | 0.0000 | 0.0000 |
| **CoCl2** | 0.0625 | 0.0022 | 0.0624 | 0.0000 | 0.0624 | 0.0624 | 0.0625 | 0.0000 | 0.0000 |
| **CuCl2** | 0.0312 | 0.0011 | 0.0312 | 0.0000 | 0.0312 | 0.0312 | 0.0312 | 0.0000 | 0.0000 |
| **FeCl3(aq)** | 0.4997 | 0.0176 | 0.4996 | 0.0001 | 0.4996 | 0.4996 | 0.4996 | 0.0000 | 0.0000 |
| **HCl(aq)** | 1.1388 | 0.0401 | 1.1385 | 0.0003 | 1.1385 | 1.1385 | 1.1388 | 0.0000 | 0.0000 |
| **Impurities** | 523.1070 | 18.4144 | 522.9632 | 0.1438 | 522.963 | 522.963 | 523.1070 | 0.0000 | 0.0000 |
| **Acetate Salt** | 1244.788 | 43.8191 | 1244.446 | 0.3422 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| **Potassium Cat** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 12469.3 | 12469.3 | 12469.26 | 0.0000 | 0.0000 |
| **Succinate Salt** | 29759.56 | 1047.597 | 29751.37 | 8.1823 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| **K2CO3** | 22.4014 | 0.7886 | 22.3952 | 0.0062 | 22.3952 | 22.3952 | 22.3952 | 0.0000 | 0.0000 |
| **K2HPO4** | 783.1917 | 27.5700 | 782.9764 | 0.2153 | 782.976 | 782.976 | 782.9764 | 0.0000 | 0.0000 |
| **KH2PO4** | 519.3898 | 18.2836 | 519.2470 | 0.1428 | 519.247 | 519.247 | 519.2470 | 0.0000 | 0.0000 |
| **MgSO4(aq)** | 30.8353 | 1.0855 | 30.8268 | 0.0085 | 30.8268 | 30.8268 | 30.8268 | 0.0000 | 0.0000 |
| **Succinic Anion** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 17775.6 | 17775.6 | 17775.64 | 0.0000 | 0.0000 |
| **Water** | 214832.8 | 23323.50 | 214614.5 | 218.282 | 214615 | 214615 | 214614.5 | 836010.32 | 97358.03 |

Table S5: Pure glycerol Section 300(a) stream table (2).

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-054** | **S-056** | **S-057** | **S-058** | **S-059** | **S-060** | **S-061** | **S-062** |
| **Mass Flowrate (MT/batch)** | 47.337 | 14.142 | 33.194 | 183.617 | 47.653 | 183.617 | 47.653 | 183.617 |
| **Temperature (οC)** | 50.3 | 50.3 | 50.3 | 26.4 | 40.4 | 26.4 | 40.4 | 37.0 |
| **Pressure (bar)** | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **(NH4)2HPO4** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 546.9287 |
| **Acetic Anion** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 748.7344 | 0.0000 |
| **CaCl2** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 1.9340 |
| **CoCl2** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0624 |
| **CuCl2** | 0.0000 | 10923.53 | 10923.53 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0312 |
| **FeCl3(aq)** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.4996 |
| **HCl(aq)** | 0.0000 | 4063.634 | 4063.634 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 3895.4598 |
| **ΝaΟΗ(aq)** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 8717.08 | 8717.08 | 0.0000 | 8019.7097 |
| **Impurities** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 522.9632 | 0.0000 |
| **Acetate Salt** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| **Potassium Cation** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 12469.255 |
| **Succinate Salt** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| **K2CO3** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 22.3952 |
| **K2HPO4** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 782.9764 |
| **KH2PO4** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 519.2470 |
| **MgSO4(aq)** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 30.8268 |
| **Succinic Anion** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 17775.64 | 0.0000 |
| **Water** | 200492.7 | 169.3183 | 97527.35 | 491606 | 8717.08 | 209210 | 214614.5 | 777542.49 |

Table S6: Pure glycerol Section 300(b) stream table.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-051** | **S-055** | **S-063** | **S-064** | **S-065** | **S-066** | **S-067** | **S-068** | **S-069** | **S-070** | **S-071** | **S-072** | **S-073** |
| **Mass Flowrate (MT/batch)** | 8360.10 | 46.553 | 233.662 | 233.662 | 233.662 | 11.809 | 1.027 | 12.835 | 34.745 | 233.139 | 47.077 | 1011.583 | 14.118 |
| **Temperature (οC)** | 25.0 | 25.0 | 52.1 | 52.1 | 60.0 | 25.0 | 25.0 | 25.0 | 25.0 | 60.0 | 25.0 | 25.0 | 25.0 |
| **Pressure (bar)** | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **Acetic Acid** | 0.0000 | 0.0000 | 761.4134 | 761.4134 | 761.4134 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 761.4134 | 0.0000 | 0.0000 | 0.0000 |
| **Impurities** | 0.0000 | 0.0000 | 522.9632 | 522.9632 | 522.9632 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 522.9632 | 0.0000 | 0.0000 |
| **NaOH(aq)** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 513.415 | 513.415 | 0.0000 | 0.0000 | 472.3415 | 0.0000 | 0.0000 |
| **Succinic Acid** | 0.0000 | 0.0000 | 18081.88 | 18081.88 | 18081.88 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 18081.883 | 0.0000 | 0.0000 | 0.0000 |
| **Water** | 836010.3 | 46553.80 | 214295.6 | 214295.6 | 214295.6 | 11808.5 | 513.415 | 12322.0 | 34745.27 | 214295.57 | 46081.462 | 1011583.3 | 14118.519 |

Table S7: Pure glycerol Section 400(a) stream table.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-074** | **S-075** | **S-076** | **S-077** | **S-078** | **S-079** | **S-080** | **S-081** | **S-082** | **S-083** | **S-084** | **S-085** | **S-086** | **S-087** | **S-088** |
| **Mass Flowrate (MT/batch)** | 258.830 | 258.830 | 258.830 | 44.102 | 139.184 | 139.184 | 75.544 | 75.544 | 0.0000 | 75.544 | 214.728 | 214.728 | 214.728 | 44.102 | 44.102 |
| **Temperature (οC)** | 54.8 | 54.8 | 95.0 | 80.0 | 114.4 | 60.0 | 80.0 | 60.0 | 60.0 | 60.0 | 60.0 | 60.1 | 25.0 | 34.0 | 4.0 |
| **Pressure (bar)** | 1.013 | 1.013 | 1.013 | 1.013 | 1.169 | 1.169 | 0.473 | 0.450 | 0.450 | 1.450 | 1.169 | 6.169 | 6.169 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **Acetic Acid** | 972.644 | 972.6441 | 972.6441 | 360.0695 | 397.0637 | 397.064 | 215.511 | 215.511 | 0.0000 | 215.5110 | 612.5747 | 612.5747 | 612.5747 | 360.0695 | 360.0695 |
| **Succinic Acid** | 18765.2 | 19877.0 | 19877.0 | 19877.0 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 4377.2094 | 1164.8335 |
| **Succinic Acid Crystals** | 1111.78 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 15499.786 | 18712.162 |
| **Water** | 237980 | 237980 | 237980 | 23865 | 138787.1 | 138787 | 75328.3 | 75328.3 | 0.0000 | 75328.327 | 214115.46 | 214115.46 | 214115.46 | 23864.834 | 23864.834 |

Table S8: Pure glycerol Section 400(b) stream table (1).

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-088** | **S-089** | **S-090** | **S-091** | **S-092** | **S-093** | **S-094** | **S-095** | **S-096** |
| **Mass Flowrate (MT/batch)** | 44.102 | 44.102 | 14.119 | 22.057 | 15.218 | 20.946 | 0.016 | 10.473 | 10.473 |
| **Temperature (οC)** | 4.0 | 4.0 | 15.0 | 10.8 | 10.8 | 4.0 | 4.5 | 4.0 | 4.0 |
| **Pressure (bar)** | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **Acetic Acid** | 360.0695 | 360.0695 | 0.0000 | 1.6435 | 64.0356 | 294.3904 | 0.0000 | 147.1952 | 147.1952 |
| **Nitrogen** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 12.4394 | 0.0000 | 0.0000 |
| **Oxygen** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 3.7764 | 0.0000 | 0.0000 |
| **Succinic Acid** | 1164.8335 | 1164.8335 | 0.0000 | 5.3168 | 207.1567 | 952.3600 | 0.0000 | 476.1800 | 476.1800 |
| **Succinic Acid Crystals** | 18712.1615 | 18712.1615 | 0.0000 | 17506.8258 | 1018.2141 | 187.1216 | 0.0000 | 93.5608 | 93.5608 |
| **Water** | 23864.8344 | 23864.8344 | 14118.519 | 4542.7725 | 13928.8537 | 19511.727 | 0.0000 | 9755.8635 | 9755.8635 |

Table S9: Pure glycerol Section 400(b) stream table (2).

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-097** | **S-098** | **S-099** | **S-100** | **S-101** | **S-102** | **S-103** | **S-104** | **S-105** |
| **Mass Flowrate (MT/batch)** | 10.473 | 195.358 | 195.358 | 55.453 | 139.905 | 55.849 | 10.473 | 143.123 | 18.436 |
| **Temperature (οC)** | 4.0 | 25.0 | 27.4 | 27.4 | 27.4 | 35.0 | 4.0 | 70.0 | 35.0 |
| **Pressure (bar)** | 2.013 | 1.013 | 1.033 | 1.033 | 1.033 | 1.013 | 2.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **Acetic Acid** | 147.1952 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 147.1952 | 0.0000 | 1.6435 |
| **Nitrogen** | 0.0000 | 149862.6999 | 149862.6999 | 42538.7560 | 107323.944 | 42538.756 | 0.0000 | 107323.94 | 0.0000 |
| **Oxygen** | 0.0000 | 45495.4121 | 45495.4121 | 12913.9421 | 32581.4700 | 12913.942 | 0.0000 | 32581.470 | 0.0000 |
| **Succinic Acid** | 476.1800 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 476.1800 | 0.0000 | 0.0000 |
| **Succinic Acid Crystals** | 93.5608 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 93.5608 | 0.0000 | 17512.1426 |
| **Water** | 9755.8635 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 396.4637 | 9755.8635 | 3224.5305 | 921.7782 |

Table S10: Crude glycerol Section 100 stream table.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **S-001** | **S-002** | **S-003** | **S-004** | **S-005** | **S-006** | **S-007** | **S-008** | **S-009** | **S-010** | **S-011** | **S-012** | **S-013** | **S-014** |
| **Mass Flowrate (MT/batch)** | 48.776 | 48.776 | 48.776 | 48.776 | 6.607 | 33.360 | 13.605 | 48.777 | 47.653 | 183.617 | 18.206 | 4.273 | 47.653 | 54548.4696 |
| **Temperature (οC)** | 25.0 | 25.0 | 50.0 | 50.3 | 25.0 | 25.0 | 25.0 | 25.0 | 37.0 | 37.0 | 25.0 | 25.0 | 40.4 | 25.2 |
| **Pressure (bar)** | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **Glycerol** | 36582.5 | 36582.45 | 36582.45 | 36582.5 | 0.0000 | 0.0000 | 0.0000 | 36582.453 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 36582.4532 | 0.0000 |
| **Impurities** | 487.766 | 487.7660 | 487.7660 | 487.766 | 0.0000 | 0.0000 | 0.0000 | 487.7660 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 487.7660 | 0.0000 |
| **Salts** | 0.0000 | 0.0000 | 0.0000 | 0.0364 | 0.0282 | 0.0364 | 0.0282 | 0.0364 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| **HCl(aq)** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 275.7607 | 0.0000 | 275.7607 | 0.0000 | 0.0000 | 264.2707 |
| **NaOH(aq)** | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 591.5454 | 0.0000 | 591.5454 | 0.0000 | 544.2218 |
| **Salt Anions** | 0.0000 | 0.0000 | 0.0000 | 591.990 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 591.9896 |
| **Salt Cations** | 0.0000 | 0.0000 | 0.0000 | 383.543 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 383.5425 |
| **Water** | 10730.9 | 10730.85 | 10730.85 | 10730.9 | 6606.77 | 33360.6 | 13605.54 | 10730.853 | 11.4900 | 591.5454 | 6618.2577 | 14197.089 | 10730.8529 | 52764.4451 |



Figure S1: Water recycle loop section from SuperPro Designer™ environment.

Table S11: Water recycle loop section stream table.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter** | **WR-001** | **WR-002** | **WR-003** | **WR-004** | **WR-005** | **WR-006** | **WR-007** | **WR-008** | **WR-009** | **WR-010** | **WR-011** | **WR-012** | **WR-013** | **WR-014** |
| **Mass Flowrate (MT/batch)** | 213.708 | 183.155 | 30.553 | 877.556 | 1060.710 | 1060.710 | 1060.319 | 0.391 | 832.476 | 150.568 | 9.828 | 53.329 | 14.118 | 14.118 |
| **Temperature (οC)** | 25.0 | 26.3 | 26.3 | 25.0 | 25.2 | 35.0 | 35.0 | 35.0 | 35.0 | 35.0 | 35.0 | 35.0 | 35.0 | 15.0 |
| **Pressure (bar)** | 6.013 | 6.013 | 6.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 | 1.013 |
| **Component Mass Flowrate (kg/batch)** |
| **Acetic Acid** | 612.4127 | 0.0000 | 612.4127 | 0.0000 | 0.0000 | 0.0000 | 215.511 | 215.511 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| **Water** | 213096 | 183154.77 | 29941.190 | 877555.56 | 1060710.3 | 1060710 | 75328.3 | 75328.3 | 0.0000 | 1060319.2 | 391.1718 | 832476.35 | 14117.54 | 14117.54 |

Table S12: Fermentation reactions stoichiometry.

|  |  |
| --- | --- |
| - | **Conversion**  |
| **Biomass Growth from Glucose (Mass Stoichiometry)**2 (NH4)2HPO4 + 80 C6H12O6 +10 (C6H12O6)2 + 8 (C6H12O6)3 + 2 (C6H12O6)n  + 1 K2HPO4 + 1 KH2PO4 + 96 O2 $\rightarrow $ 40 Biomass + 140 CO2 + 20 H2O |  75%  |
| **Succinic Acid Production from Glucose (Mass Stoichiometry)**150 C6H12O6 +3 (C6H12O6)2 + 2 (C6H12O6)3 + 40 CO2 $\rightarrow $ 150 C4H6O4 + 3 C2H4O2 + 2 Impurities + 40 H2O |  100% |
| **Biomass Growth from Glycerol (Mass Stoichiometry)**2 (NH4)2HPO4 + 100 C3H8O3 + 1 K2HPO4 + 1 KH2PO4 + 96 O2 $\rightarrow $40 Biomass + 140 CO2 + 20 H2O | 75% |
| **Succinic Acid Production from Glycerol (Mass Stoichiometry)**270 C3H8O3 $\rightarrow $ 190 C4H6O4 + 8 C2H4O2 + 5 Impurities + 67 H2O | 100% |
| **Succinic Acid Neutralization (Molar Stoichiometry)**K2CO3 + C4H6O4 $\rightarrow $ C4H4K2O4 + H2O |  100%  |
| **Acetic Acid Neutralization (Molar Stoichiometry)**K2CO3 + 2 C2H4O2 $\rightarrow $ 2 C2H3KO2 + CO2 + H2O |  100%  |

Figure S2: *Tornado diagrams for the influence of various input parameters to the NPV and PBT for the crude glycerol (a) and glucose (b) case.*