

|                             |                                                                                                                                                                                                                                                                                                                                                                                                                  |
|-----------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Title                       | Optimization of surfactant addition in cellulosic ethanol process using integrated techno-economic and life cycle assessment for bioprocess design                                                                                                                                                                                                                                                               |
| Authors                     | Kadhum, Haider Jawad;Rajendran, Karthik;Murthy, Ganti S.                                                                                                                                                                                                                                                                                                                                                         |
| Publication date            | 2018-10-04                                                                                                                                                                                                                                                                                                                                                                                                       |
| Original Citation           | Kadhum, H. J., Rajendran, K. and Murthy, G. S. (2018) 'Optimization of surfactant addition in cellulosic ethanol process using integrated techno-economic and life cycle assessment for bioprocess design', ACS Sustainable Chemistry and Engineering, 6(11), pp. 13687-13695. doi:10.1021/acssuschemeng.8b00387                                                                                                 |
| Type of publication         | Article (peer-reviewed)                                                                                                                                                                                                                                                                                                                                                                                          |
| Link to publisher's version | 10.1021/acssuschemeng.8b00387                                                                                                                                                                                                                                                                                                                                                                                    |
| Rights                      | © 2018, American Chemical Society. This document is the Accepted Manuscript version of a Published Work that appeared in final form in ACS Sustainable Chemistry and Engineering after technical editing by the publisher. To access the final edited and published work see <a href="https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.8b00387">https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.8b00387</a> |
| Download date               | 2026-08-31 18:09:57                                                                                                                                                                                                                                                                                                                                                                                              |
| Item downloaded from        | <a href="https://hdl.handle.net/10468/7155">https://hdl.handle.net/10468/7155</a>                                                                                                                                                                                                                                                                                                                                |



# UCC

**University College Cork, Ireland**  
Coláiste na hOllscoile Corcaigh

# **Optimization of Surfactant Addition in Cellulosic Ethanol Process Using Integrated Techno-Economic and Life Cycle Assessment for Bioprocess Design**

Haider Jawad Kadhum <sup>a,b,§</sup>, Karthik Rajendran <sup>a,c,d,§</sup>, Ganti S. Murthy <sup>a,\*</sup>

<sup>a</sup> Department of Biological and Ecological Engineering, Oregon State University, Corvallis OR-97331, United States

<sup>b</sup> College of Agriculture, Al-Qasim Green University, Babylon, Iraq

<sup>c</sup> Environmental Research Institute, MaREI centre, University College Cork, Cork, Ireland

<sup>d</sup> School of Engineering, University College Cork, Cork, Ireland

*§ Both the authors had contributed equally to this manuscript*

Emails: kadhumh@oregonstate.edu; karthik.1988@gmail.com, k.rajendran@ucc.ie;  
Ganti.Murthy@oregonstate.edu

\*Corresponding author:

Ganti.Murthy@oregonstate.edu

Phone: +1 (541) 737 6291

Fax: +1 (541) 737 2082

**Supplementary 2:**



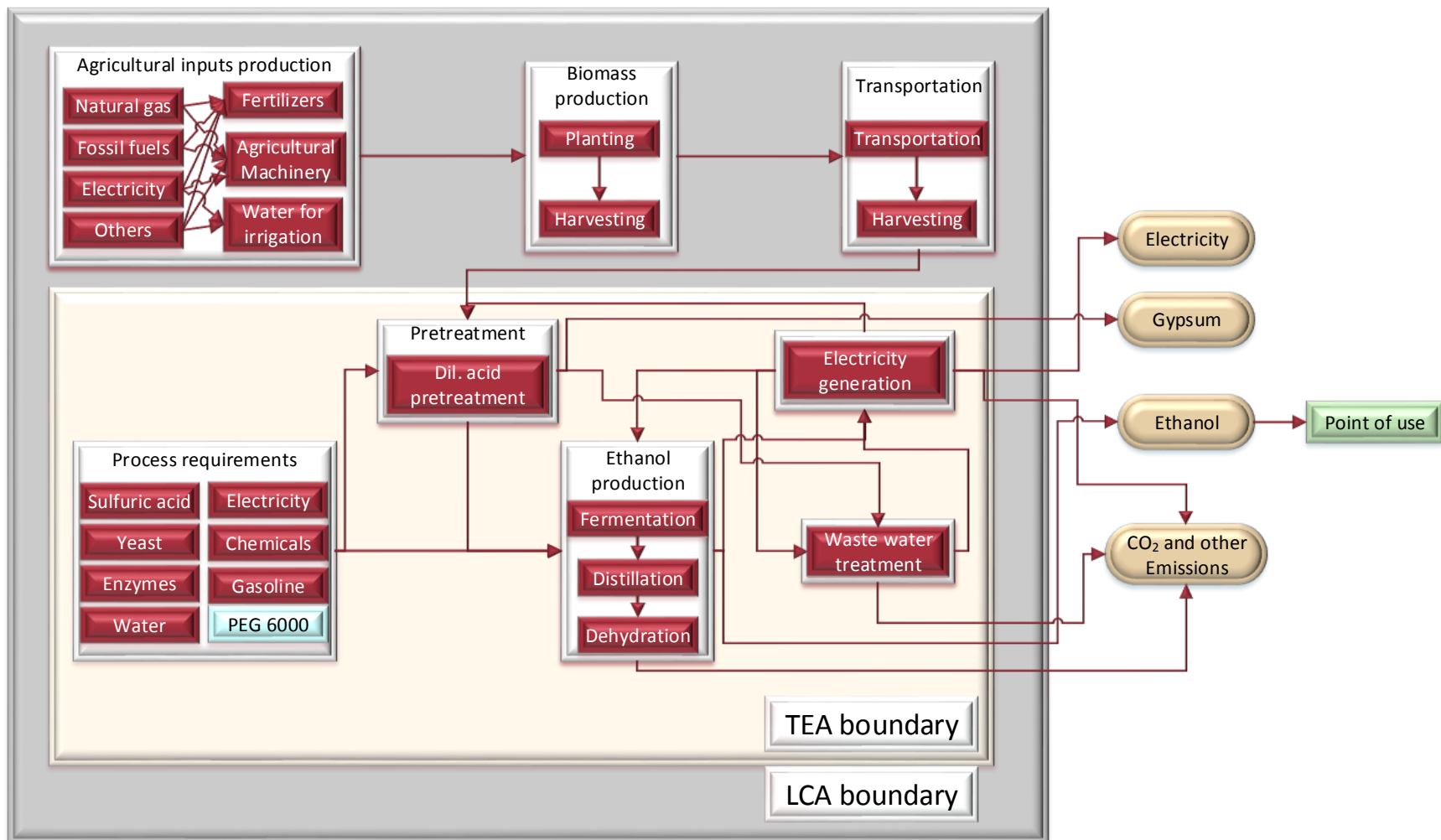


Figure S2-S2. System boundary description highlighting the boundary for techno-economic analysis and life cycle assessments.

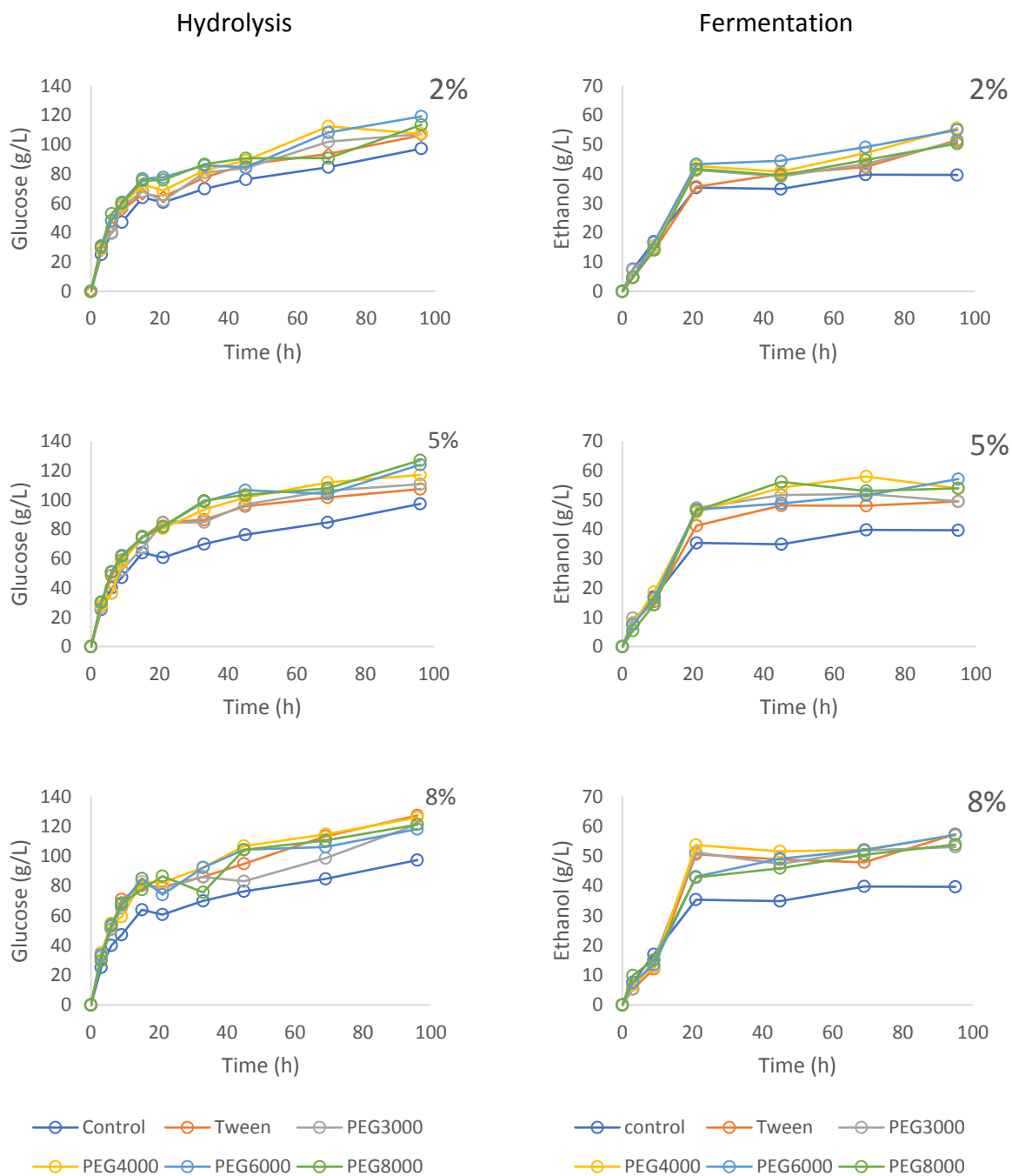


Figure S2-S3. Effect of glucose and ethanol release for various surfactants at various concentrations.

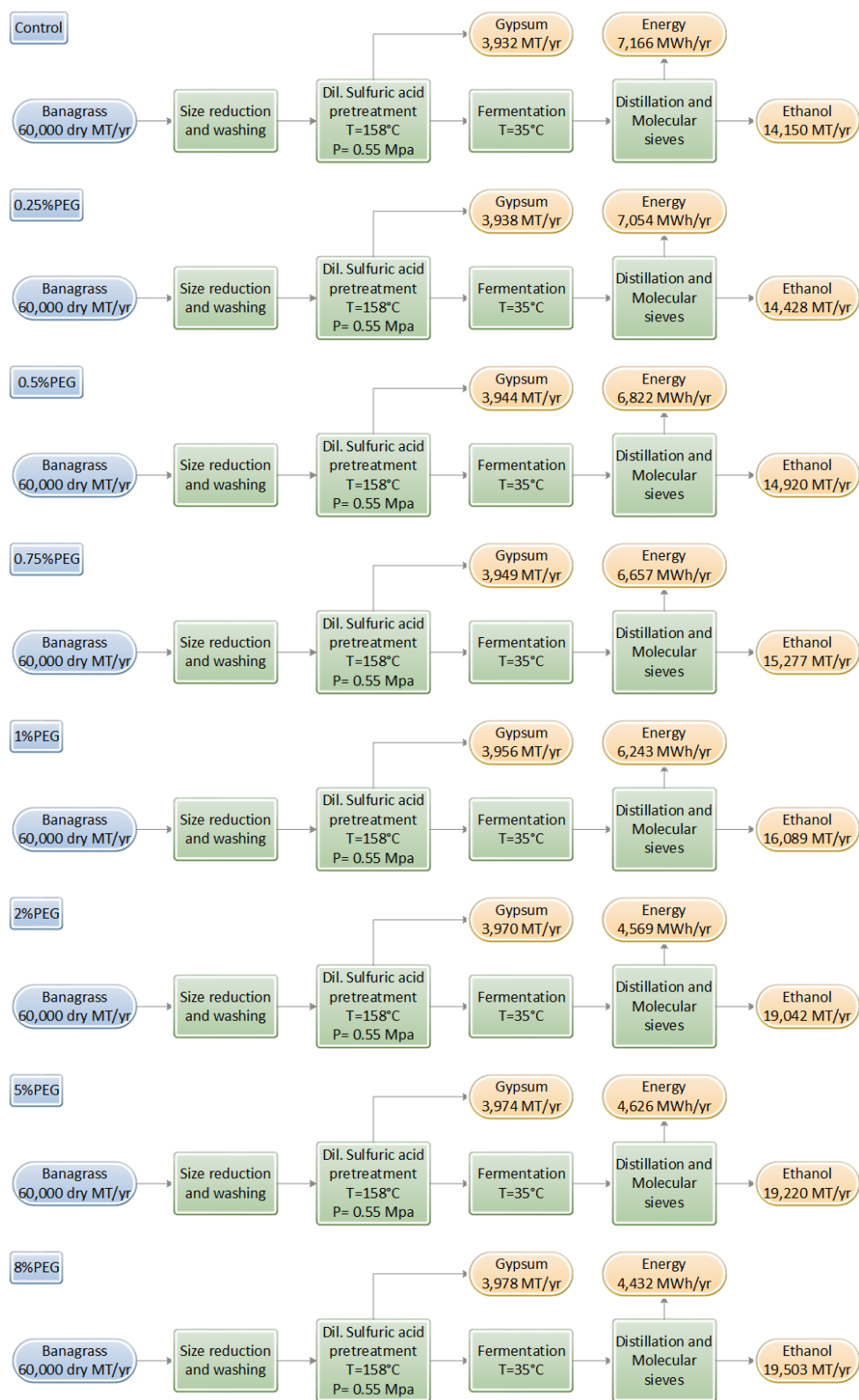


Figure S2-S4. Overall mass balance for different scenarios using a different concentration of PEG6000 and control.

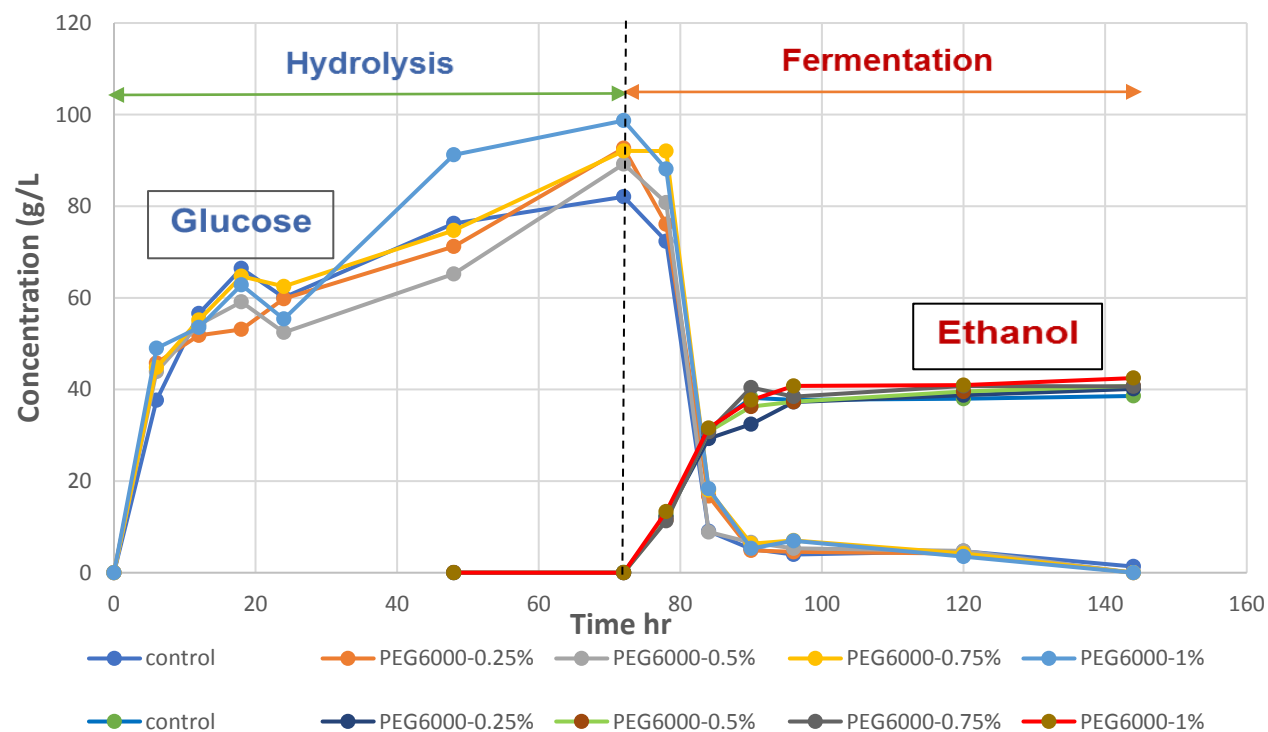


Figure S2-S5. Glucose and ethanol release at lower concentrations (<1%) using PEG6000.

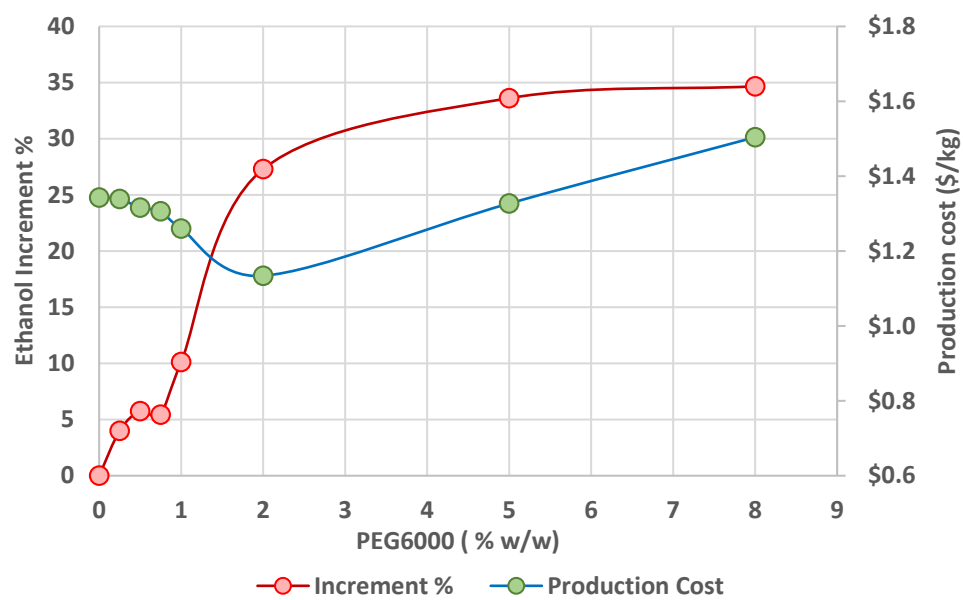


Figure S2-S6. Percentage of ethanol increment compared to control vs PEG concentration





Figure S2-S7. Life cycle assessment impact metrics for the experiments at various PEG6000 concentrations.

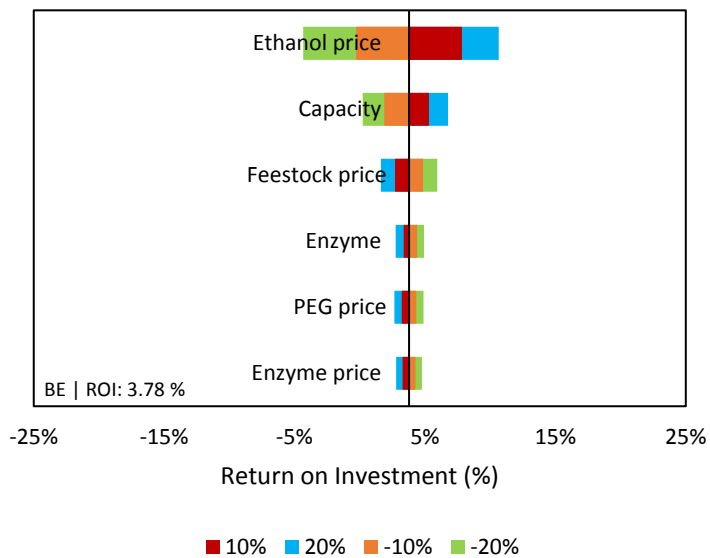


Figure S2-S8: Sensitivity analysis based on the techno-economic evaluation for the optimized process (PEG 6000 2%).

Table S2-S1. The experimental design used in this study.

First experiment.

| Factors       | Type  | Level | Values                                              |
|---------------|-------|-------|-----------------------------------------------------|
| Surfactant    | Fixed | 5     | PEG 3000, PEG 4000, PEG 6000, PEG8000, and Tween 80 |
| Concentration | Fixed | 4     | 0%, 2%, 5% and 8%                                   |

Second experiment.

| Factors                   | Level | Values                        |
|---------------------------|-------|-------------------------------|
| PEG 6000<br>Concentration | 5     | 0%, 0.25%, 0.5% ,0.75% and 1% |

Table S2-S2. Hydrolysis and fermentation parameters used to implement simulation.

|               | Glucose g/L | Ethanol g/L |
|---------------|-------------|-------------|
| Control       | 82.1        | 38.0        |
| PEG6000-0.25% | 92.7        | 38.8        |
| PEG6000-0.5%  | 89.2        | 39.5        |
| PEG6000-0.75% | 92.1        | 40.8        |
| PEG6000-1%    | 98.7        | 40.9        |
| PEG6000-2%    | 108.2       | 49.1        |

Table S2-S3. Raw materials used in TEA and LCA scenarios.

|                   | Unit (MT) |         |          |         |          |         |
|-------------------|-----------|---------|----------|---------|----------|---------|
|                   | Control   | 2%PEG   | 0.25%PEG | 0.5%PEG | 0.75%PEG | 1%PEG   |
| Water             | 149,820   | 145,920 | 149,250  | 148,650 | 148,170  | 147,470 |
| Gasoline          | 130       | 180     | 140      | 140     | 150      | 150     |
| Calcium hydroxide | 1,800     | 1,820   | 1,800    | 1,800   | 1,810    | 1,810   |
| Sulfuric acid     | 2,630     | 2,650   | 2,630    | 2,630   | 2,640    | 2,640   |
| Biomass (dry MT)  | 60,000    | 60,000  | 60,000   | 60,000  | 60,000   | 60,000  |
| Cellulase         | 4,260     | 4,260   | 4,260    | 4,260   | 4,260    | 4,260   |
| DAP               | 20        | 20      | 20       | 20      | 20       | 20      |
| Yeast             | 50        | 50      | 50       | 50      | 50       | 50      |
| PEG               | 0         | 1,400   | 200      | 400     | 500      | 700     |

*\*The values mentioned above were rounded off to the nearest 10 metric tons.*

Table S2-S4. Utilities consumed, and electricity power produced at various PEG 6000 concentrations.

|                          | Control     | 2%PEG       | 0.25%PEG    | 0.5%PEG     | 0.75%PEG    | 1%PEG       |
|--------------------------|-------------|-------------|-------------|-------------|-------------|-------------|
| Power Consumption (kW-h) | (6,863,000) | (6,879,000) | (6,865,000) | (6,867,000) | (6,868,000) | (6,869,000) |
| Power Production (KW-h)  | 14,029,000  | 11,448,000  | 13,919,000  | 13,689,000  | 13,525,000  | 13,112,000  |
| Steam (MT)               | (158,000)   | (167,000)   | (159,000)   | (160,000)   | (161,000)   | (162,000)   |
| Cooling Water (MT)       | 9,648,000   | 11,140,000  | 9,738,000   | 9,890,000   | 10,000,000  | 10,240,000  |
| Chilled Water (MT)       | 1,466,000   | 1,227,000   | 1,456,000   | 1,435,000   | 1,420,000   | 1,382,000   |
| CT Water (MT)            | 6,588,000   | 6,600,000   | 6,590,000   | 6,592,000   | 6,594,000   | 6,598,000   |
| Steam High P (MT)        | (26,000)    | (27,000)    | (26,000)    | (26,000)    | (26,000)    | (26,000)    |

*\*The value inside the parentheses indicates that it was produced on site.*

Table S2-S5. Monte Carlo Analysis of the LCA results (2% PEG addition)\*

| Run | Acidification | Ecotoxicity | Eutrophication | Global Warming | Human Health - carcinogenics | Human Health - non-carcinogenics | Ozone Depletion | Photochemical ozone formation | Resource depletion - fossil fuels | Respiratory effects |
|-----|---------------|-------------|----------------|----------------|------------------------------|----------------------------------|-----------------|-------------------------------|-----------------------------------|---------------------|
| 1   | -1.72E-01     | -9.64E+01   | -2.53E-02      | -5.15E+01      | -4.39E-06                    | -2.07E-06                        | -4.46E-07       | -2.38E+00                     | -2.57E+02                         | -9.41E-03           |
| 2   | -5.77E-02     | 2.27E+02    | -2.52E-02      | -2.78E+01      | 1.26E-06                     | -9.30E-07                        | 1.49E-06        | -1.60E+00                     | -1.52E+02                         | -2.78E-02           |
| 3   | -7.35E-02     | 3.00E+00    | -7.93E-03      | -1.93E+01      | -1.29E-07                    | -1.33E-07                        | -1.87E-07       | -7.47E-01                     | -8.96E+01                         | -5.31E-03           |
| 4   | -5.08E-02     | -5.20E+01   | -1.01E-02      | -1.51E+01      | -1.36E-06                    | -3.19E-06                        | -1.04E-07       | -6.91E-01                     | -7.26E+01                         | -2.41E-03           |
| 5   | -2.41E-02     | -1.92E+01   | -7.38E-03      | -5.97E+00      | -6.78E-07                    | -4.85E-07                        | -6.19E-08       | -2.72E-01                     | -2.94E+01                         | -3.20E-04           |
| 6   | -1.81E-02     | -2.19E+01   | -4.58E-03      | -5.62E+00      | -4.42E-07                    | -7.03E-07                        | -5.24E-08       | -2.68E-01                     | -2.73E+01                         | -8.74E-04           |
| 7   | -1.61E-02     | -3.27E+00   | -3.07E-03      | -5.16E+00      | -1.49E-07                    | -9.75E-08                        | -2.68E-08       | -2.45E-01                     | -2.49E+01                         | -1.02E-03           |
| 8   | -1.63E-02     | -2.79E+01   | -3.41E-03      | -4.95E+00      | -2.55E-06                    | -5.25E-07                        | -2.14E-08       | -2.32E-01                     | -2.41E+01                         | -8.62E-04           |
| 9   | -2.14E-02     | -6.41E+01   | -7.94E-03      | -4.21E+00      | -1.81E-06                    | -2.47E-06                        | -1.59E-07       | -1.77E-01                     | -1.77E+01                         | -5.95E-04           |
| 10  | -1.03E-01     | -4.33E+00   | 1.34E-02       | -3.64E+00      | -7.87E-07                    | 9.76E-07                         | -9.88E-07       | -2.38E-01                     | -2.13E+01                         | -9.06E-05           |
| 11  | -8.94E-03     | -1.85E+01   | -2.37E-03      | -2.74E+00      | -3.09E-07                    | -6.31E-07                        | -3.30E-08       | -1.26E-01                     | -1.37E+01                         | -4.10E-04           |
| 12  | -1.20E-02     | -2.54E+02   | -3.46E-03      | -2.42E+00      | -4.44E-07                    | -8.55E-06                        | -2.83E-09       | -1.07E-01                     | -1.34E+01                         | -1.28E-04           |
| 13  | -9.43E-03     | -1.32E+01   | -2.14E-03      | -2.38E+00      | -2.13E-07                    | -7.09E-07                        | 1.30E-08        | -6.18E-02                     | -1.34E+01                         | 4.07E-04            |
| 14  | -8.68E-03     | -1.95E+01   | -4.97E-03      | -2.20E+00      | -3.21E-07                    | -1.15E-06                        | -1.32E-08       | -9.44E-02                     | -1.12E+01                         | -2.01E-04           |

|    |           |           |           |           |           |           |           |           |           |           |
|----|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 15 | -1.13E-02 | 2.61E+00  | -1.42E-03 | -2.07E+00 | 3.28E-08  | 1.10E-06  | -2.10E-08 | -1.34E-01 | -1.99E+01 | -3.60E-04 |
| 16 | -5.59E-03 | -6.29E+00 | -1.20E-03 | -1.94E+00 | -4.13E-08 | -1.79E-07 | -3.13E-08 | -9.70E-02 | -9.52E+00 | -4.71E-04 |
| 17 | -7.02E-03 | -4.21E+00 | -8.37E-03 | -1.82E+00 | -2.32E-07 | -2.40E-07 | -2.08E-08 | -8.85E-02 | -1.01E+01 | -1.78E-04 |
| 18 | -5.03E-03 | -3.94E+00 | -2.67E-03 | -1.27E+00 | -1.69E-07 | -1.12E-07 | -1.09E-08 | -6.04E-02 | -6.69E+00 | -9.54E-05 |
| 19 | -6.75E-03 | -1.89E+01 | -3.49E-03 | -1.11E+00 | -5.63E-07 | -4.19E-07 | -2.90E-08 | -4.92E-02 | -5.16E+00 | -6.10E-05 |
| 20 | -3.50E-03 | -1.80E+00 | -3.80E-04 | -9.90E-01 | -1.30E-07 | -1.86E-08 | -5.41E-09 | -4.77E-02 | -5.08E+00 | -1.52E-04 |
| 21 | -3.27E-03 | -1.54E+00 | -4.84E-04 | -9.80E-01 | -5.11E-08 | -3.28E-08 | -1.80E-08 | -4.75E-02 | -4.93E+00 | -1.94E-04 |
| 22 | -1.40E-02 | 1.64E+01  | 3.58E-03  | -9.57E-01 | 4.95E-07  | 3.58E-07  | -9.24E-08 | -5.61E-02 | -1.56E+00 | -1.28E-03 |
| 23 | -3.08E-03 | -3.28E+00 | -1.13E-03 | -8.53E-01 | -1.06E-07 | -9.11E-08 | -2.75E-09 | -4.02E-02 | -4.45E+00 | -1.27E-04 |
| 24 | -4.92E-03 | -5.49E+00 | -3.01E-03 | -8.09E-01 | -3.58E-07 | -2.10E-06 | -1.18E-08 | -3.11E-02 | -4.78E+00 | 9.12E-05  |
| 25 | -2.01E-03 | -2.03E+00 | -6.07E-04 | -7.83E-01 | -7.31E-08 | -5.66E-08 | 7.88E-10  | -4.10E-02 | -4.30E+00 | -1.08E-04 |
| 26 | -2.09E-03 | -6.04E+00 | -8.22E-04 | -5.85E-01 | -1.49E-07 | -2.02E-07 | 2.58E-10  | -2.60E-02 | -3.40E+00 | 1.27E-05  |
| 27 | -1.56E-03 | -3.76E-01 | -3.34E-03 | -5.81E-01 | -2.36E-07 | 5.10E-08  | 2.56E-08  | -2.32E-02 | -4.28E+00 | 1.71E-04  |
| 28 | -1.30E-03 | 3.44E+00  | 1.49E-04  | -5.10E-01 | -4.14E-08 | 1.41E-07  | -2.00E-08 | -2.83E-02 | -2.85E+00 | -1.29E-04 |
| 29 | -3.65E-03 | -7.77E+00 | -2.12E-03 | -4.21E-01 | -6.13E-08 | -4.68E-07 | 3.81E-08  | 2.80E-02  | -3.38E+00 | 8.07E-04  |
| 30 | 4.63E-02  | -8.08E-03 | 2.64E-03  | -3.70E-01 | -1.99E-08 | 9.79E-09  | -1.97E-08 | 1.67E+00  | -2.02E+00 | 2.76E-04  |
| 31 | 9.48E-03  | -2.17E+01 | -3.89E-02 | -3.59E-01 | -5.59E-07 | -3.39E-07 | 8.55E-08  | 6.02E-03  | -6.42E+00 | 1.26E-03  |
| 32 | -2.19E-03 | -4.89E+00 | -7.87E-04 | -3.23E-01 | -1.13E-07 | -2.28E-07 | 1.67E-09  | -1.45E-02 | -2.32E+00 | 1.81E-04  |
| 33 | -2.26E-03 | -4.67E+00 | -5.51E-04 | -3.14E-01 | -1.01E-07 | -4.26E-07 | -2.81E-09 | -1.35E-02 | -1.80E+00 | -6.46E-06 |
| 34 | -1.60E-03 | 4.63E+00  | -1.17E-03 | -2.75E-01 | -2.72E-08 | 1.73E-07  | -4.68E-08 | -2.53E-02 | -1.42E+00 | -1.96E-04 |
| 35 | -1.61E-03 | -3.98E+00 | -4.31E-04 | -2.63E-01 | -9.24E-08 | -1.81E-06 | 3.37E-09  | -1.19E-02 | -1.68E+00 | 3.61E-05  |
| 36 | -2.93E-03 | -1.15E+01 | 2.06E-03  | -2.31E-01 | -5.62E-07 | -3.75E-07 | -1.62E-08 | -4.41E-03 | -2.29E+00 | 3.68E-04  |
| 37 | -7.09E-04 | 1.71E+00  | -2.41E-04 | -2.16E-01 | 7.42E-08  | -9.05E-09 | 2.33E-08  | -1.28E-02 | -1.18E+00 | -2.92E-04 |
| 38 | -2.00E-03 | -6.86E+00 | -1.14E-03 | -2.00E-01 | -2.51E-07 | -4.31E-07 | 1.11E-09  | -2.18E-03 | -1.45E+00 | 1.59E-04  |
| 39 | -2.07E-04 | -9.47E-01 | -2.80E-04 | -1.95E-01 | -4.33E-08 | -9.07E-09 | 6.48E-09  | -1.12E-02 | -1.46E+00 | 1.35E-05  |
| 40 | -1.46E-03 | -5.74E+00 | -1.30E-04 | -1.71E-01 | -7.02E-08 | -9.73E-08 | -9.48E-09 | -8.36E-03 | -1.21E+00 | 7.23E-05  |
| 41 | -1.38E-03 | -1.09E+01 | -8.37E-04 | -1.70E-01 | -1.29E-07 | -4.62E-07 | -9.30E-09 | -7.48E-03 | -1.43E+00 | 5.06E-05  |
| 42 | -2.36E-03 | -4.69E-02 | -2.63E-04 | -1.54E-01 | -4.05E-09 | -2.57E-08 | -1.45E-08 | -1.11E-02 | -6.89E-01 | -1.07E-04 |
| 43 | -4.20E-04 | 4.78E-01  | 7.59E-05  | -1.39E-01 | -1.50E-08 | 1.36E-08  | 2.94E-09  | -7.80E-03 | -1.13E+00 | 2.00E-05  |
| 44 | -2.89E-03 | -8.16E-01 | -1.89E-04 | -1.30E-01 | -2.30E-08 | -2.47E-09 | -5.16E-08 | -2.67E-02 | -3.46E-01 | -8.92E-05 |
| 45 | -3.12E-05 | -2.64E+00 | -6.67E-04 | -6.53E-02 | -4.17E-08 | -7.30E-08 | 8.91E-09  | -3.12E-03 | -9.36E-01 | 9.65E-05  |
| 46 | -2.11E-04 | 1.31E+01  | -3.00E-04 | -6.40E-02 | 6.06E-08  | -3.17E-08 | -5.84E-08 | -3.18E-03 | -9.04E-01 | 6.54E-05  |

|    |           |           |           |           |           |           |           |           |           |           |
|----|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 47 | 1.13E-03  | 2.27E+00  | -1.57E-04 | -6.23E-02 | 1.31E-08  | 1.53E-07  | 4.80E-09  | -1.67E-02 | -7.53E-01 | -3.82E-04 |
| 48 | -7.73E-04 | 1.34E-01  | 7.28E-05  | -4.82E-02 | 1.19E-08  | 1.54E-08  | -4.73E-09 | -5.71E-03 | -5.18E-01 | 1.35E-05  |
| 49 | -1.49E-03 | -5.56E+00 | 5.13E-04  | -4.53E-02 | -1.34E-07 | -1.74E-06 | -1.63E-08 | -1.44E-02 | -7.08E-02 | -1.90E-04 |
| 50 | 1.58E-04  | -7.10E-01 | -1.55E-04 | -3.47E-02 | -1.56E-08 | -1.64E-08 | 4.39E-09  | -4.10E-03 | -7.52E-01 | 3.05E-05  |
| 51 | -1.31E-03 | 2.68E+00  | 3.46E-05  | -3.36E-02 | 1.79E-08  | 3.95E-08  | -2.11E-08 | -3.55E-03 | -5.07E-01 | 1.28E-04  |
| 52 | -4.10E-04 | -2.57E+00 | -4.06E-04 | -3.23E-02 | -3.92E-08 | -7.02E-08 | -4.10E-09 | -4.75E-03 | -6.06E-01 | 6.82E-05  |
| 53 | -7.78E-04 | -4.40E-01 | 5.73E-06  | -2.35E-02 | -1.31E-08 | 7.25E-09  | -9.90E-09 | -6.89E-03 | -3.89E-01 | 7.65E-05  |
| 54 | -2.34E-04 | -3.06E-01 | -9.69E-05 | -1.88E-02 | -9.91E-09 | 1.10E-09  | -8.17E-09 | -8.84E-03 | -1.35E-01 | 7.72E-06  |
| 55 | -9.00E-04 | 2.76E-01  | 2.10E-04  | -1.80E-02 | -9.31E-09 | 2.38E-07  | -1.26E-08 | -9.10E-03 | -2.66E-01 | 2.04E-05  |
| 56 | -2.45E-04 | -4.77E-01 | -8.38E-05 | -1.46E-02 | -6.24E-09 | -1.62E-08 | 1.07E-09  | -4.20E-03 | -4.47E-01 | -9.09E-06 |
| 57 | 4.65E-03  | 3.13E+01  | 2.92E-03  | 5.48E-03  | 4.23E-07  | 9.78E-07  | 1.23E-08  | -1.35E-02 | 1.57E-01  | -2.69E-04 |
| 58 | -5.10E-04 | -2.11E+00 | -2.35E-04 | 1.20E-02  | -6.79E-08 | -4.87E-08 | -3.43E-09 | -3.59E-03 | -2.65E-01 | 4.24E-06  |
| 59 | 7.97E-04  | 1.85E+00  | 9.34E-05  | 1.64E-02  | 2.65E-08  | -4.07E-08 | 7.07E-09  | 1.57E-02  | -6.48E-01 | -3.71E-05 |
| 60 | -1.46E-03 | -2.88E+00 | -9.98E-04 | 1.82E-02  | 1.54E-07  | -1.43E-06 | -6.97E-09 | -9.37E-03 | -1.06E-01 | -1.82E-05 |
| 61 | -1.34E-03 | -3.85E+00 | 1.79E-04  | 2.01E-02  | -1.95E-08 | 1.43E-08  | -1.48E-08 | -1.14E-03 | -7.08E-02 | 1.93E-04  |
| 62 | -8.57E-05 | -1.59E-01 | -6.32E-05 | 2.37E-02  | -1.92E-10 | -3.34E-08 | 2.13E-09  | -1.82E-03 | -3.30E-01 | 2.62E-05  |
| 63 | -1.49E-03 | -1.00E+01 | -9.05E-04 | 2.69E-02  | -2.55E-07 | -3.00E-07 | -7.86E-09 | 1.95E-04  | -8.65E-02 | 5.91E-05  |
| 64 | 3.02E-04  | -5.76E-01 | -1.15E-04 | 2.74E-02  | -1.18E-08 | -1.26E-08 | 1.86E-09  | -1.46E-03 | -4.03E-01 | 4.67E-05  |
| 65 | -4.80E-05 | -9.21E-01 | -3.68E-06 | 3.04E-02  | -2.27E-08 | -2.98E-08 | -1.94E-09 | -5.63E-04 | -3.76E-01 | 1.18E-04  |
| 66 | 3.70E-04  | -5.78E-01 | 3.77E-06  | 3.19E-02  | -8.14E-09 | -7.20E-09 | 4.52E-09  | -2.82E-03 | -5.98E-01 | 5.33E-05  |
| 67 | -6.42E-05 | 1.28E-01  | 1.22E-04  | 3.49E-02  | 1.74E-09  | 1.08E-08  | 6.53E-10  | -1.28E-03 | -2.79E-01 | 2.88E-05  |
| 68 | -1.72E-04 | -1.22E+00 | -1.12E-04 | 4.32E-02  | -2.51E-08 | -1.24E-08 | -2.84E-09 | -9.25E-03 | -4.17E-02 | 3.49E-06  |
| 69 | -4.69E-04 | -2.40E+00 | -3.32E-05 | 4.66E-02  | -4.20E-09 | -2.03E-07 | -2.35E-09 | -3.60E-03 | -1.56E-02 | -2.82E-05 |
| 70 | 1.21E-04  | 1.43E-01  | 1.10E-04  | 5.38E-02  | 1.54E-08  | 6.23E-08  | -1.86E-10 | -9.54E-04 | -1.75E-01 | 2.86E-05  |
| 71 | -1.87E-05 | 7.15E-01  | 3.04E-05  | 6.17E-02  | 5.01E-09  | 3.91E-08  | 9.18E-10  | -3.07E-03 | -2.39E-03 | -6.27E-06 |
| 72 | 4.87E-05  | -1.47E-02 | 4.06E-05  | 6.44E-02  | 3.16E-10  | -1.97E-09 | 1.17E-09  | 7.19E-05  | -6.05E-02 | 2.54E-06  |
| 73 | -1.64E-04 | 1.40E+00  | 6.82E-04  | 7.36E-02  | 3.85E-08  | 4.97E-08  | -2.13E-09 | 1.77E-04  | -6.91E-03 | 2.44E-05  |
| 74 | 7.31E-04  | 9.04E-01  | 2.62E-04  | 7.58E-02  | 2.74E-08  | 2.04E-08  | 1.48E-08  | 1.63E-02  | -2.99E-01 | 5.48E-05  |
| 75 | -4.93E-04 | -4.47E+00 | -9.39E-04 | 7.66E-02  | -1.55E-07 | -9.04E-08 | 1.18E-09  | 6.55E-04  | 3.51E-02  | 7.74E-05  |
| 76 | -1.04E-04 | 2.36E-01  | 5.28E-05  | 7.79E-02  | -4.59E-09 | 1.42E-08  | -1.67E-09 | -2.45E-03 | -3.77E-01 | 3.98E-05  |
| 77 | -2.47E-05 | -1.24E+00 | 2.31E-04  | 7.96E-02  | -2.18E-08 | -1.54E-08 | -3.97E-09 | -4.43E-03 | 1.82E-01  | -9.71E-06 |
| 78 | -2.66E-04 | -1.45E-01 | 3.10E-06  | 7.97E-02  | -4.88E-09 | 1.02E-08  | -4.40E-09 | -6.97E-05 | -2.17E-02 | 5.89E-05  |



|     |           |           |           |          |           |           |           |           |           |           |
|-----|-----------|-----------|-----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 79  | 1.87E-04  | 2.47E+00  | 2.68E-06  | 7.97E-02 | 9.43E-08  | 6.05E-08  | -7.71E-10 | -4.62E-03 | 5.95E-03  | -9.97E-06 |
| 80  | 5.22E-05  | 8.26E-02  | 1.01E-04  | 8.00E-02 | 8.62E-09  | 8.02E-09  | 1.16E-09  | -3.53E-04 | 2.00E-02  | -2.17E-06 |
| 81  | 1.46E-03  | -6.16E-01 | -6.52E-05 | 8.31E-02 | -1.51E-08 | -6.43E-08 | 8.78E-09  | -5.77E-04 | -4.03E-01 | 4.65E-05  |
| 82  | 1.63E-05  | 4.85E-01  | 1.97E-04  | 8.49E-02 | 8.41E-09  | 3.08E-08  | 4.00E-09  | -5.34E-03 | -1.33E+00 | 4.58E-05  |
| 83  | -1.04E-05 | -2.86E-01 | -7.15E-06 | 8.51E-02 | -1.86E-09 | 3.39E-09  | -1.27E-09 | 1.03E-03  | 1.61E-02  | 4.22E-05  |
| 84  | 5.36E-04  | -3.18E-01 | -8.36E-05 | 8.65E-02 | -1.68E-08 | -1.57E-08 | 6.51E-09  | 1.18E-03  | -1.91E-01 | 6.68E-05  |
| 85  | 1.77E-04  | 1.96E+00  | -1.17E-05 | 8.88E-02 | -2.46E-08 | 5.56E-08  | -1.78E-08 | -1.02E-02 | 1.50E-02  | 3.19E-05  |
| 86  | 2.64E-04  | 1.93E+00  | 8.00E-04  | 8.95E-02 | 4.96E-08  | 5.39E-07  | 5.00E-09  | -2.52E-04 | 8.22E-02  | -4.13E-05 |
| 87  | 4.86E-04  | 1.66E+00  | 2.30E-04  | 9.18E-02 | 4.30E-08  | 7.71E-08  | 6.53E-09  | 1.41E-03  | 7.52E-02  | 2.89E-06  |
| 88  | -9.53E-05 | 5.87E+00  | 5.69E-04  | 9.27E-02 | 7.16E-09  | 7.31E-07  | 4.26E-08  | -1.24E-03 | 4.71E-02  | -1.19E-04 |
| 89  | 6.22E-04  | -1.28E+00 | -1.09E-04 | 9.59E-02 | -3.66E-08 | -1.61E-08 | 1.05E-08  | 1.38E-03  | -1.67E-01 | 7.37E-05  |
| 90  | 2.61E-04  | 4.77E-01  | 4.94E-05  | 1.00E-01 | 2.05E-08  | 3.19E-08  | 1.88E-09  | 1.51E-03  | 5.45E-02  | 3.08E-05  |
| 91  | 4.97E-04  | -2.23E+00 | -8.76E-03 | 1.06E-01 | -1.04E-07 | -6.41E-08 | 4.94E-09  | -1.30E-02 | 4.69E-01  | 4.29E-05  |
| 92  | 2.88E-03  | 1.83E+01  | 3.24E-03  | 1.07E-01 | 3.33E-07  | 3.71E-07  | 5.28E-08  | 6.30E-02  | 5.89E-01  | 8.71E-03  |
| 93  | 2.11E-04  | -3.03E-01 | -1.85E-04 | 1.10E-01 | -5.41E-09 | -1.85E-08 | 3.29E-09  | 2.26E-03  | 4.85E-02  | 4.19E-05  |
| 94  | 3.60E-04  | -2.96E-01 | 1.46E-04  | 1.12E-01 | -3.08E-09 | 2.17E-09  | 1.76E-09  | 2.25E-03  | 5.43E-02  | 6.25E-05  |
| 95  | 8.21E-04  | -3.79E-02 | 1.25E-04  | 1.20E-01 | 1.03E-08  | 4.01E-08  | 5.79E-09  | 1.58E-03  | -3.77E-02 | 3.81E-05  |
| 96  | 3.08E-04  | 5.10E-01  | 3.42E-05  | 1.21E-01 | 5.64E-09  | 2.65E-09  | 6.66E-09  | 5.02E-03  | 1.55E-02  | 3.73E-05  |
| 97  | 6.59E-04  | 3.47E+00  | 3.14E-04  | 1.23E-01 | 3.98E-08  | 1.11E-07  | 2.85E-09  | 7.19E-04  | 1.17E-01  | -9.76E-06 |
| 98  | 1.05E-03  | 3.19E+00  | -1.12E-03 | 1.29E-01 | 1.50E-08  | 1.08E-07  | 7.42E-09  | 2.73E-03  | 1.70E-01  | 4.65E-05  |
| 99  | 1.81E-03  | -9.84E-01 | -2.32E-04 | 1.41E-01 | -5.30E-09 | -1.82E-08 | 1.68E-08  | 3.14E-03  | -1.10E-01 | 1.13E-04  |
| 100 | 5.06E-04  | 3.55E+00  | 3.75E-04  | 1.44E-01 | 5.05E-08  | 2.42E-07  | 4.68E-09  | 2.58E-03  | 3.89E-01  | -2.01E-05 |
| 101 | 2.66E-06  | -2.82E+00 | -4.49E-04 | 1.53E-01 | -1.26E-07 | -2.75E-07 | 2.89E-09  | 5.65E-03  | 5.15E-02  | 1.49E-04  |
| 102 | 4.22E-04  | -1.98E+00 | 2.31E-04  | 1.68E-01 | 4.60E-08  | 6.37E-08  | 2.00E-08  | 4.16E-04  | 3.57E-01  | -3.23E-05 |
| 103 | 7.58E-04  | 6.44E+00  | 1.29E-03  | 1.74E-01 | 9.57E-08  | 2.03E-07  | 7.02E-09  | 9.98E-03  | 4.62E-01  | -4.59E-05 |
| 104 | 7.82E-04  | 1.82E-01  | 1.47E-04  | 1.76E-01 | 2.20E-08  | 8.29E-09  | 9.57E-11  | -2.25E-03 | 5.55E-01  | 6.43E-05  |
| 105 | -5.25E-03 | 1.51E+01  | 4.99E-03  | 1.81E-01 | 3.01E-07  | 4.54E-07  | -5.52E-08 | 1.44E-03  | -4.13E-01 | -1.86E-04 |
| 106 | 1.35E-03  | -9.98E+00 | 3.66E-03  | 1.98E-01 | -2.60E-07 | -5.20E-07 | 8.03E-08  | 1.37E-01  | -4.26E+00 | 3.70E-05  |
| 107 | -6.65E-05 | 1.38E+00  | 5.02E-04  | 1.99E-01 | 6.46E-08  | 4.25E-08  | -1.67E-09 | 4.18E-03  | 6.52E-01  | -2.05E-05 |
| 108 | 1.14E-03  | 1.51E+00  | 4.89E-04  | 2.00E-01 | 6.59E-08  | 3.75E-08  | 1.28E-08  | 2.94E-02  | 1.95E-01  | 5.73E-05  |
| 109 | 2.31E-03  | -6.43E-01 | -7.67E-04 | 2.04E-01 | 4.42E-09  | -1.98E-08 | 3.21E-08  | 5.63E-03  | 3.47E-02  | 5.49E-05  |
| 110 | 2.72E-03  | -3.53E-01 | -1.23E-05 | 2.06E-01 | -1.02E-08 | 6.19E-09  | 1.32E-08  | 2.03E-02  | 2.34E-01  | 1.16E-04  |

|               |           |           |           |          |           |           |           |           |           |           |
|---------------|-----------|-----------|-----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 111           | 1.26E-03  | 3.67E+00  | 3.65E-03  | 2.10E-01 | 9.35E-08  | 1.16E-07  | 1.08E-08  | 1.81E-03  | 1.10E-01  | 4.69E-05  |
| 112           | -1.99E-03 | -2.85E+01 | -3.20E-03 | 2.11E-01 | -4.53E-07 | -1.32E-06 | -2.01E-09 | 1.87E-02  | -1.01E-01 | 3.84E-04  |
| 113           | 2.64E-03  | 6.75E+00  | -4.92E-05 | 2.68E-01 | -2.20E-08 | 7.21E-07  | -1.54E-08 | -9.98E-03 | 3.91E-01  | -1.18E-05 |
| 114           | 8.95E-04  | -4.06E-01 | 8.17E-05  | 2.83E-01 | 1.64E-09  | 5.61E-10  | 6.15E-10  | 9.96E-03  | 9.15E-01  | 1.11E-04  |
| 115           | 1.19E-03  | 4.36E+00  | 1.35E-03  | 2.87E-01 | 1.80E-07  | 2.55E-07  | -7.29E-10 | 5.06E-03  | 1.18E+00  | -1.47E-04 |
| 116           | 1.48E-03  | -8.79E-01 | -2.61E-04 | 2.94E-01 | -8.93E-08 | 8.88E-08  | 5.19E-08  | 1.04E-02  | 2.86E-01  | 2.04E-04  |
| 117           | 1.89E-03  | 5.02E+00  | 2.79E-03  | 2.98E-01 | 1.49E-07  | 5.01E-07  | 9.59E-09  | 8.41E-03  | 1.17E+00  | -2.78E-05 |
| 118           | 7.68E-03  | -1.06E+00 | -8.01E-04 | 3.19E-01 | -4.59E-08 | -8.77E-08 | 4.20E-08  | 1.25E-02  | -6.79E-02 | 1.84E-04  |
| 119           | 4.23E-03  | -5.99E+00 | -1.88E-03 | 3.26E-01 | -2.26E-07 | -9.55E-08 | 2.99E-08  | 1.07E-02  | 1.64E-02  | 5.33E-04  |
| 120           | 2.80E-03  | -8.31E-01 | 1.24E-04  | 4.04E-01 | 4.18E-09  | -2.19E-08 | -9.00E-09 | 1.67E-02  | 1.23E+00  | 1.54E-04  |
| 121           | -8.62E-03 | 1.07E+01  | 4.00E-03  | 4.42E-01 | 4.09E-08  | 2.63E-07  | -5.51E-08 | -1.06E-01 | -1.15E+01 | -1.20E-04 |
| 122           | 2.61E-03  | 1.76E+01  | 1.83E-03  | 4.94E-01 | 4.08E-07  | 3.16E-06  | 9.71E-09  | 1.52E-02  | 2.40E+00  | -1.27E-04 |
| 123           | 8.49E-03  | 1.08E+01  | 4.97E-03  | 7.79E-01 | 2.81E-07  | 2.75E-07  | 4.45E-08  | 4.43E-02  | 6.98E-01  | 8.58E-04  |
| 124           | 8.70E-03  | -2.37E+00 | 1.79E-03  | 1.13E+00 | 3.38E-06  | 3.81E-07  | -1.97E-07 | 4.60E-02  | 4.96E+00  | 1.37E-04  |
| 125           | 3.82E-02  | -3.03E+01 | -4.03E-03 | 2.69E+00 | -7.40E-07 | -6.27E-07 | 5.19E-08  | 8.74E-02  | 8.58E+00  | 2.76E-03  |
| 126           | 2.56E-02  | 3.71E+02  | 1.21E-02  | 3.68E+00 | 2.33E-06  | 1.22E-05  | 1.50E-07  | 1.23E-01  | 9.27E+00  | 7.51E-04  |
| 127           | -9.64E-01 | -5.45E+03 | -3.92E-01 | 4.01E+00 | -2.74E-05 | -1.49E-04 | -3.55E-05 | 5.18E+00  | -8.63E+01 | 5.90E-02  |
| 128           | 3.90E-02  | 2.30E+02  | 2.34E-02  | 7.61E+00 | 2.91E-06  | 6.70E-06  | 1.61E-07  | 1.51E-01  | 1.39E+00  | 3.88E-03  |
| 129           | 5.24E-02  | 1.94E+02  | 2.22E-02  | 1.04E+01 | 4.91E-06  | 6.80E-06  | 1.29E-07  | 3.44E-01  | 4.90E+01  | -7.10E-04 |
| 130           | 3.33E-02  | 5.19E+01  | 1.56E-02  | 1.06E+01 | 7.59E-07  | 2.48E-06  | 2.70E-08  | 4.75E-01  | 4.99E+01  | 2.03E-03  |
| 131           | 9.02E-02  | 4.94E+01  | 3.29E-02  | 2.19E+01 | 4.86E-06  | 1.20E-06  | -3.45E-07 | 8.49E-01  | 1.15E+02  | 8.48E-04  |
| 132           | -2.73E-01 | -2.54E+02 | 1.18E-01  | 2.22E+01 | -2.67E-06 | -3.24E-05 | -6.25E-06 | 4.08E+00  | -3.26E+01 | 2.62E-02  |
| 133           | 1.06E-01  | 3.56E+01  | 1.80E-02  | 3.07E+01 | 1.54E-06  | 3.28E-07  | 3.15E-07  | 1.43E+00  | 1.45E+02  | 4.63E-03  |
| 134           | 1.04E-01  | 1.72E+01  | 1.35E-02  | 3.22E+01 | 5.73E-07  | 1.01E-06  | 2.28E-07  | 1.55E+00  | 1.49E+02  | 6.73E-03  |
| 135           | 1.20E-01  | 3.18E+02  | 3.50E-02  | 4.28E+01 | 2.65E-06  | 8.70E-06  | 6.50E-07  | 1.50E+00  | 1.37E+02  | 6.27E-03  |
| Average       | -9.00E-03 | -3.60E+01 | -1.82E-03 | 2.00E-01 | -1.62E-07 | -1.22E-06 | -3.05E-07 | 7.07E-02  | -2.59E+00 | 5.56E-04  |
| Std deviation | 9.07E-02  | 4.74E+02  | 3.62E-02  | 8.34E+00 | 2.55E-06  | 1.32E-05  | 3.11E-06  | 6.86E-01  | 3.82E+01  | 6.25E-03  |

\*All inputs to the bioethanol process (Biomass, cellulase enzymes, yeast, phosphate fertilizers, lime, sulphuric acid and water) were assumed to vary according to a normal distribution with a standard deviation equal to 10% of the mean value. The mean value was the same as the 2% PEG scenario described earlier.