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

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Supplementary 2:

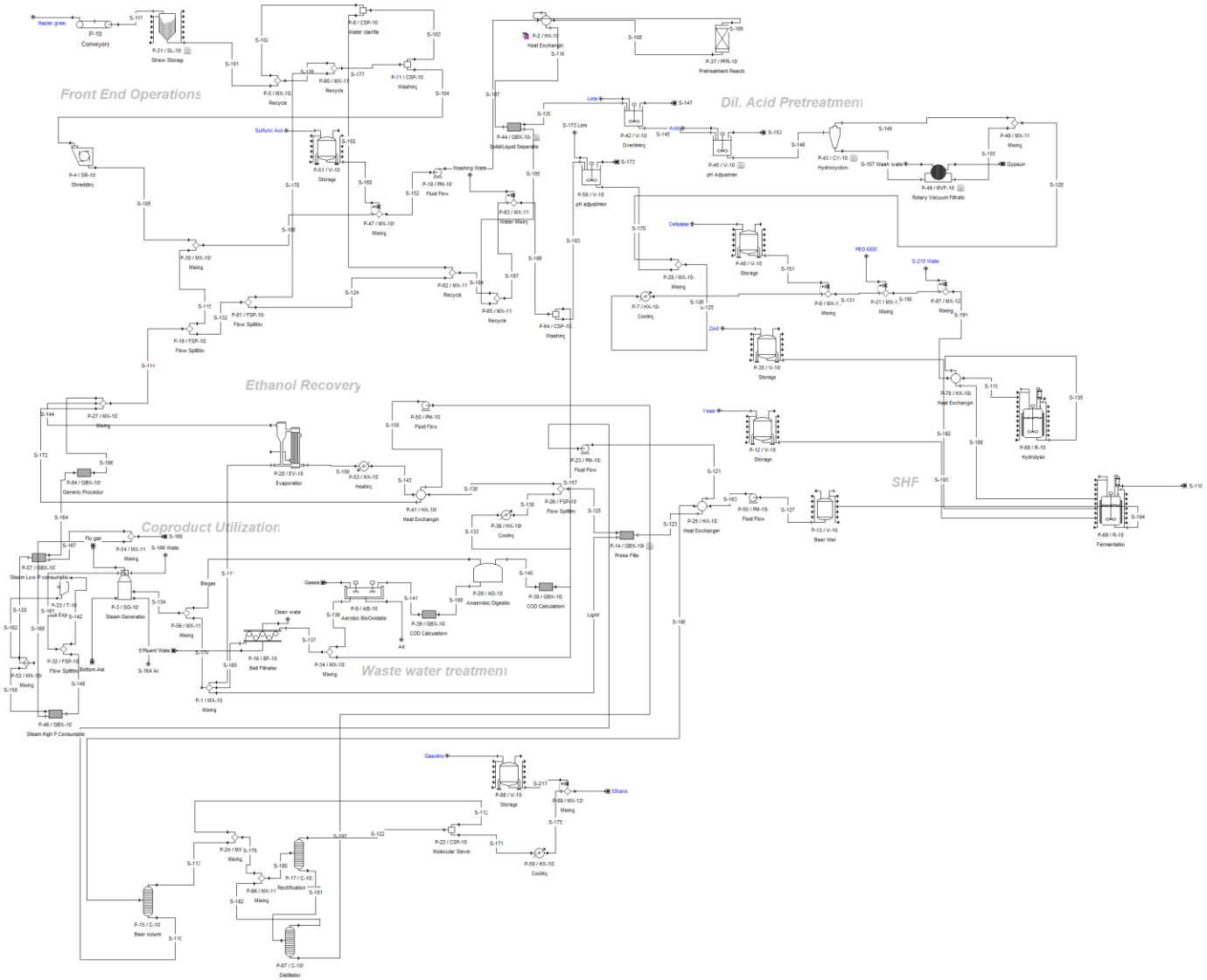


Figure S2-S1. Process flow diagram of ethanol production.

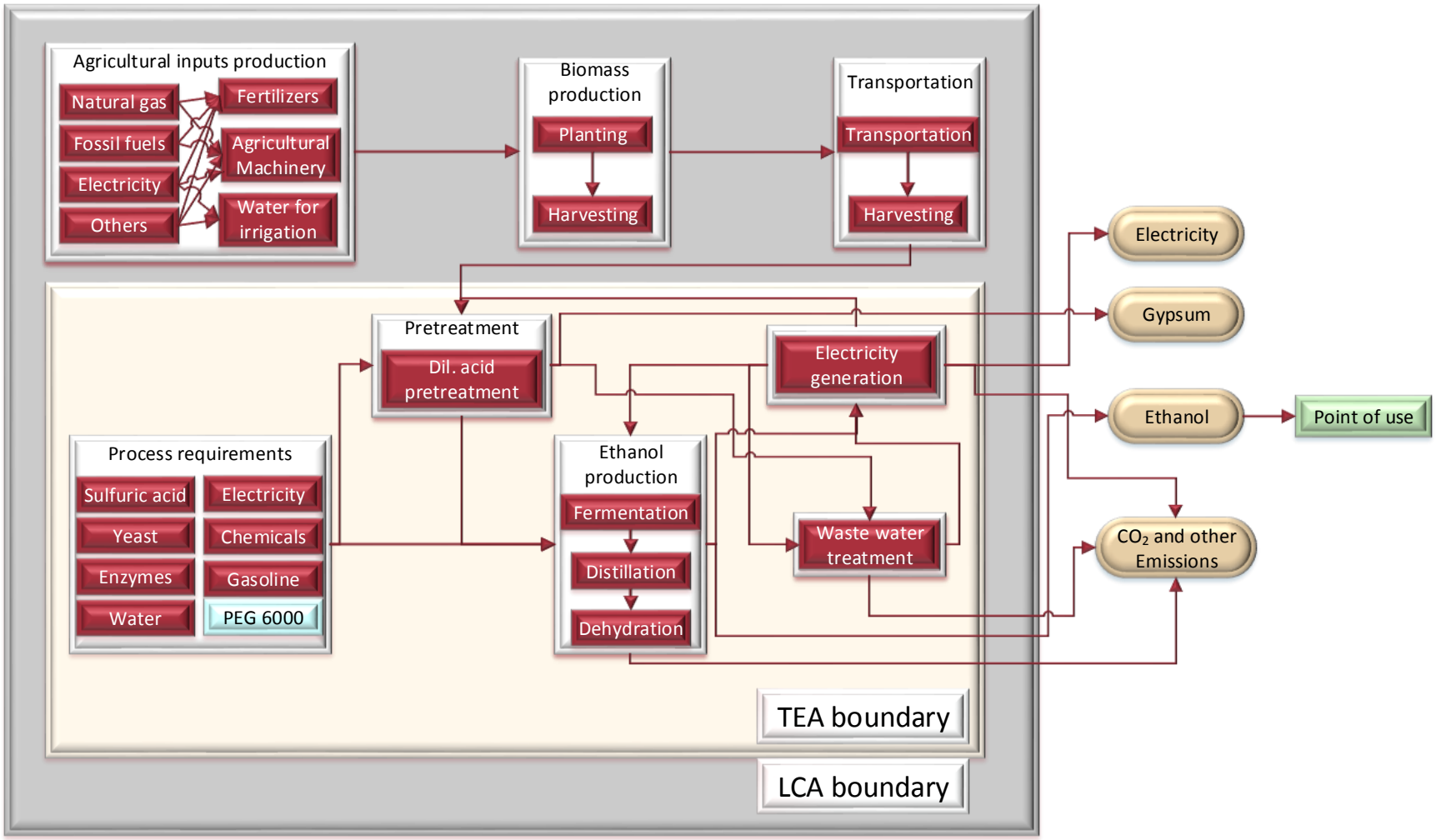


Figure S2-S2. System boundary description highlighting the boundary for techno-economic analysis and life cycle assessments.

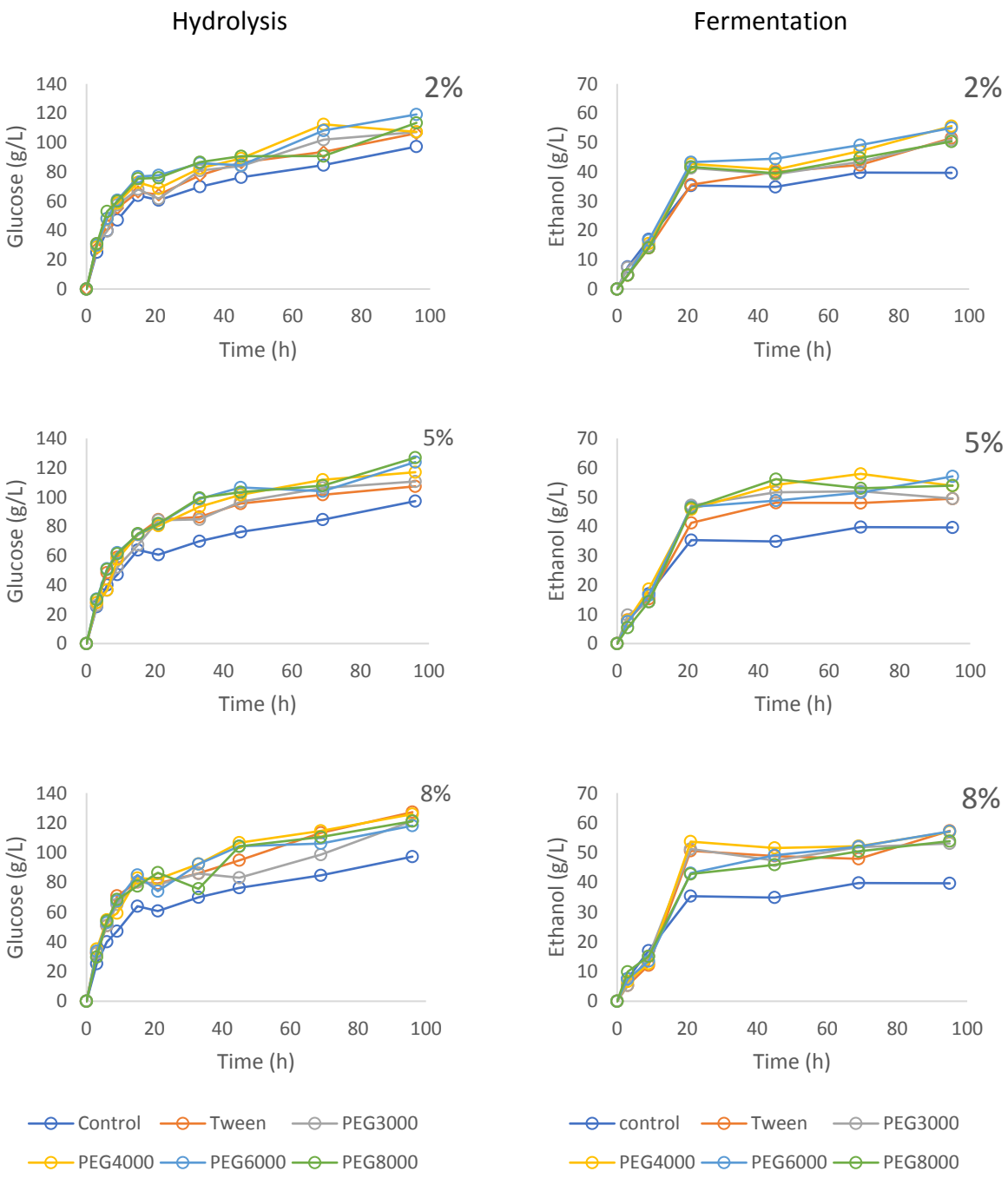


Figure S2-S3. Effect of glucose and ethanol release for various surfactants at various concentrations.

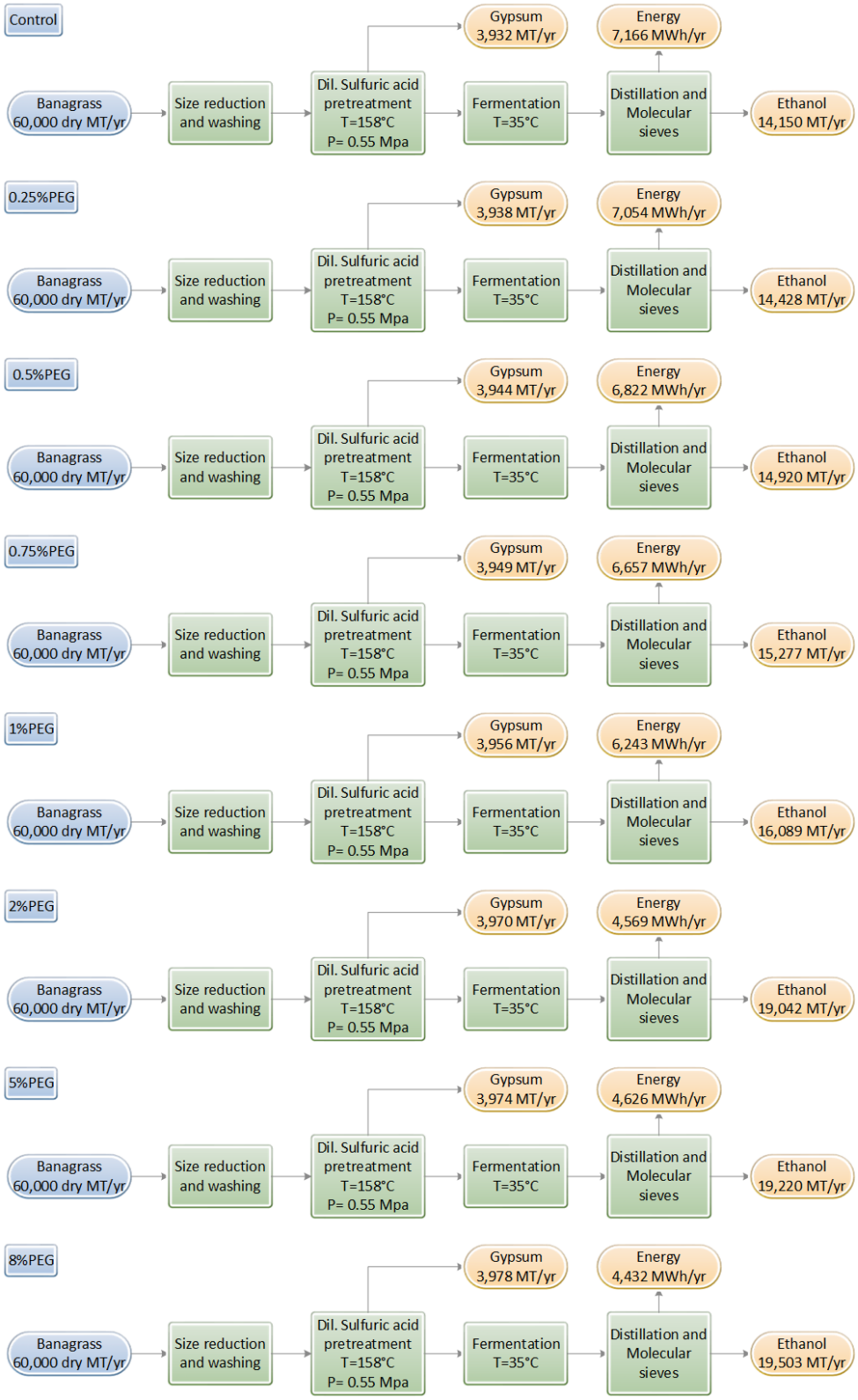


Figure S2-S4. Overall mass balance for different scenarios using a different concentration of PEG6000 and control.

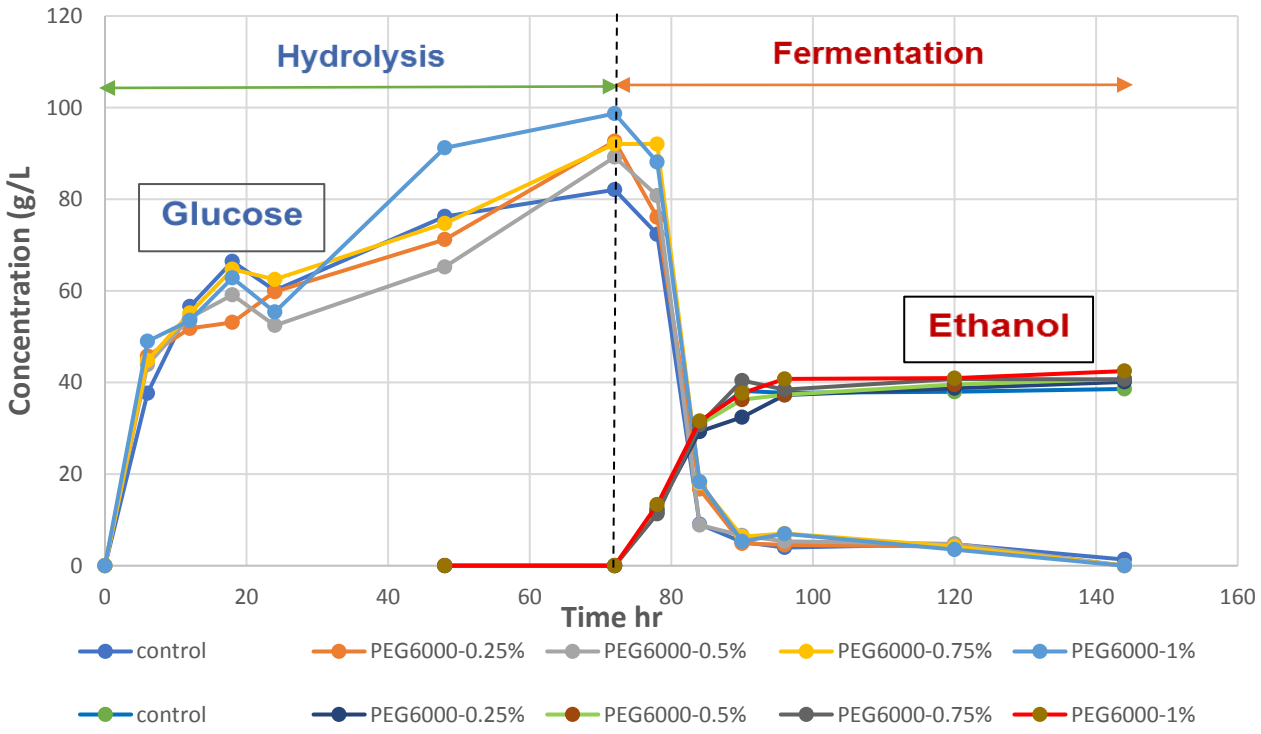


Figure S2-S5. Glucose and ethanol release at lower concentrations (<1%) using PEG6000.

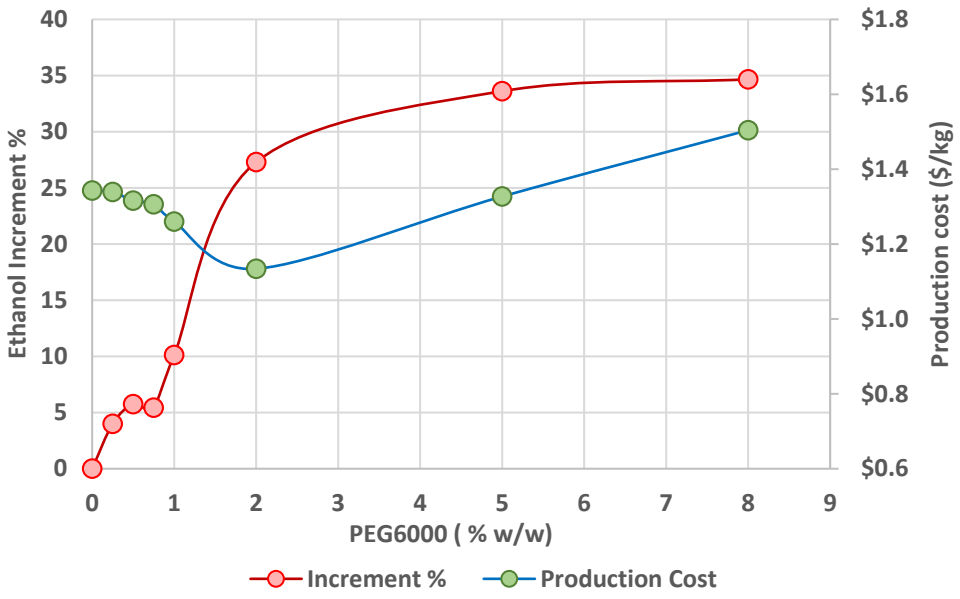


Figure S2-S6. Percentage of ethanol increment compared to control vs PEG concentration



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

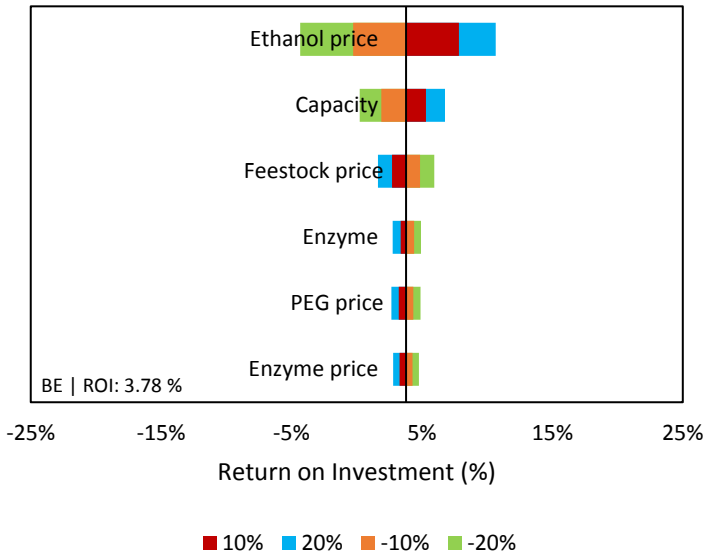


Figure S2-S8: Sensitivity analysis based on the techno-economic evaluation for the optimized process (PEG 6000 2%).

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 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
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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.