Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary Information for "Process Simulation and Economic Evaluation of the Industrial Production of Short-Chain Polyglycerol Oligomers"

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- 13 pages;

- 6 equations;

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S.1- Lang method

The methodology used to calculate the capital costs was the Lang Method, explained in detail by Seider et al.[1] To apply the method, it is necessary to estimate the f.o.b. purchase price for each piece of equipment, which are calculated by empirical equations. In addition, as these formulas were designed for another time, prices must be updated to the current time. This is done by means of the Plant Cost Index. Once this is done, all the f.o.b. prices are summed up and the result is multiplied by 1.05, to account for the delivery of the equipment to the plant site. Finally, the result must be multiplied by the appropriate Lang factor, f_L, to obtain the total fixed investment. Equation S.1 summarizes the described procedure.

$$I_F = 1.05 \times f_L \times \sum_i \left(\frac{PCI}{PCI_b}\right) C_i \quad (S.1)$$

In this equation, I_F is the fixed investment; f_L is the Lang factor; PCI is the Plant Cost Index for the project year; PCI_b is the Plant Cost Index for the base year; C_i is the f.o.b. purchase price of equipment i.

The formulas for calculating the f.o.b. process were obtained in Seider et al.[1] and refer to the year 2013, whose PCI_b value was 567. All of them were updated to the latest PCI available at the time of this analysis, for the month of September 2021, whose value was equal to 754.7.

The Lang factor takes into account the costs of installation, instrumentation and control, plumbing, electrical network, auxiliary buildings, land acquisition, construction costs, involved engineering and fees. For plants that process only fluids, the Lang factor is equal to 5.04. To obtain the total investment, the working capital, considered 15% of the total investment, must be added to the fixed investment.[1] In this work, it was assumed that the construction of the plant would take place over three years, with investments of 30%, 40% and 30% distributed over the years.

S.2- Production cost calculation

Production costs were estimated according to the methodology of Turton et al.[2] The total production cost is the cost related to the day-to-day operation of a plant, and can be divided into three categories: direct costs, indirect costs and general expenses. Direct costs include the cost of acquiring raw materials, purchasing catalysts and solvents, operating labor, technical supervision, utilities, effluent disposal, maintenance and repairs, operating supplies, laboratory charges, patents and royalties. Indirect costs include material packaging and storage, local taxes and insurance. These costs do not depend on the production level. Finally, general expenses include administrative costs, product distribution and sales, research and development.

For the material costs, the inlet/outlet flow rates were multiplied by the price of each material, and the operating labor cost is the product between the average salary of operators and the number of workers that the plant demands, calculated with Equation S.2:[2]

$$N_{OL} = \left(6.29 + 31.7{N_S}^2 + 0.23N_{NS}\right)^{0.5} \quad (\mathrm{S.2})$$

where N_{OL} is the number of workers per shift; N_S is the number of processes involving solids, which is zero in this work; N_{NS} is the number of processes that do not involve particulate solids. This count includes columns, reactors and heat exchangers. Pumps and vessels are not accounted for.[2]

The other costs are then estimated as a function of these costs and the fixed investment, according to the relations shown in Table S.1.

Table S.1. Production cost relations.[2]

Cost	Type	Relation
Technical supervision	Direct	18% of operating labor
Maintenance and repairs	Direct	6% of fixed investment
Operating supplies	Direct	15% of maintenance and repairs
Laboratory charges	Direct	15% of operating labor
Patents and royalties	Direct	3% of the total production cost
Packaging and storage	Indirect	6% of (operating labor + technical supervision + maintenance and repairs)
Local taxes	Indirect	3.2% of fixed investment
Insurance	Indirect	0.5% of fixed investment
Administrative costs	General expense	15% de (operating labor + technical supervision + maintenance and repairs)
Product distribution and sale	General expense	11% of the total production cost
Research and development	General expense	5% of the total production cost

S.3- Additional modeling considerations

S.3.1- Reaction phase definition

In the simulator, reaction phase was chosen as "overall" because, although the reaction is known to be processed in the liquid phase, the authors do not seem to have considered only the volume of this phase in the kinetic model proposition, but the entire reactor volume. This assumption arose because, during the simulations, when "combined liquid" was chosen as reaction phase, it was not possible to obtain conversions above 69%.

S.3.2- Calculation of non-glycerol inlet flow rates

For the calculation of the mass flow rates of water, catalyst and argon that enter the process, it was necessary to divide the average mass flow of glycerol produced by a plant, that is, 1,558.65 kg/h, by the mass of glycerol used by Richter et al.,[3] which is 0.05 kg. The result (31,172.99) is the ratio factor by which the article quantities were multiplied, resulting in 15.54 kg/h for water and 50.05 kg/h for argon. The amount of catalyst was stablished as 0.4% of the glycerol mass, resulting in 6.23 kg/h.

S.4- Stream property tables

Table S.2. Process streams for the maximum diglycerol production configuration.

Stream	Glycerol Inlet	Glycerol Recycle	Argon Inlet	Argon Recycle	Water
Temperature (°C)	25	25	25	25	25
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	0	0	1	1	0
Flow rate (kg/h)	1559	1687	0.1257	104.1	32.36
Enthalpy (kcal/kg)	-1761	-1761	-	-5.591×10^{-2}	-3780
Mass fractions					
Glycerol	0.9990	0.9990	0.0000	0.0000	0.0000
Argon	0.0000	0.0000	1.0000	1.0000	0.0000
Water	0.0010	0.0010	0.0000	0.0000	0.0000
Cesium bicarbonate	0.0000	0.0000	0.0000	0.0000	0.0000
Diglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Triglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000
Stream	**Catalyst**	**Glycerol**	**Argon**	**Water + Catalyst**	**1**
Temperature (°C)	25	25	25	25	260
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	0	0	1	0	0
Flow rate (kg/h)	12.99	3246	104.2	45.35	3246
Enthalpy (kcal/kg)	-1005	-1761	-	-2985	-1601
Mass fractions					
Glycerol	0.0000	0.9990	0.0000	0.0000	0.9990
Argon	0.0000	0.0000	1.0000	0.0000	0.0000
Water	0.0000	0.0010	0.0000	0.7136	0.0010
Cesium bicarbonate	1.0000	0.0000	0.0000	0.2864	0.0000
Diglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Triglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000
Stream	**2**	**3**	**4**	**5**	**6**
Temperature (°C)	260	260	260	260	105
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	1	1	1	0	0
Flow rate (kg/h)	104.2	45.35	776.3	2619	616.2
Enthalpy (kcal/kg)	29.20	-2322	-1551	-986.9	-2039
Mass fractions					
Glycerol	0.0000	0.0000	0.5774	0.4717	0.7273
Argon	1.0000	0.0000	0.1341	0.0000	0.0000
Water	0.0000	0.7136	0.2283	0.0041	0.2043
Cesium bicarbonate	0.0000	0.2864	0.0160	0.0002	0.0126
Diglycerol	0.0000	0.0000	0.0442	0.5239	0.0557
Triglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000

Table S.2. Process streams for the maximum diglycerol production configuration (continuation).

Stream	**7**	**8**	**9**	**10**	**11**
Temperature (°C)	105	0	0	0	0
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	1	1	0	1	0
Flow rate (kg/h)	160.1	104.4	55.72	104.1	0.2904
Enthalpy (kcal/kg)	-1024	-11.42	-3575	-3.173	-3552
Mass fractions					
Glycerol	0.0004	0.0000	0.0011	0.0000	0.0000
Argon	0.6502	0.9972	0.0000	1.0000	0.0000
Water	0.3208	0.0025	0.9170	0.0000	0.9089
Cesium bicarbonate	0.0287	0.0003	0.0819	0.0000	0.0911
Diglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Triglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000
Stream	**12**	**13**	**14**	**15**	**16**
Temperature (°C)	25	209.8	254.1	254.1	254.1
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	1	0.1493	1	0	0.2747
Flow rate (kg/h)	104.1	3235	351.0	2884	3235
Enthalpy (kcal/kg)	-5.591×10^{-2}	-1187	-1953	-1045	-1143
Mass fractions					
Glycerol	0.0000	0.5204	0.5920	0.5117	0.5204
Argon	1.0000	0.0000	0.0003	0.0000	0.0000
Water	0.0000	0.0422	0.3493	0.0061	0.0434
Cesium bicarbonate	0.0000	0.0026	0.0215	0.0003	0.0026
Diglycerol	0.0000	0.4347	0.0366	0.4588	0.4130
Triglycerol	0.0000	0.0000	0.0003	0.0094	0.0084
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0137	0.0122
Stream	**17**	**18**	**19**	**20**	**21**
Temperature (°C)	185.7	165.0	53.08	193.2	185.4
Pressure (kPa)	3	3	3	3	3
Vapor fraction	0.5338	0.3157	1	0	1
Flow rate (kg/h)	3235	3235	148.9	3086	1683
Enthalpy (kcal/kg)	-1143	-1197	-3036	-1109	-1462
Mass fractions					
Glycerol	0.5204	0.5204	0.0005	0.5455	1.0000
Argon	0.0000	0.0000	0.0008	0.0000	0.0000
Water	0.0434	0.0434	0.9423	0.0000	0.0000
Cesium bicarbonate	0.0026	0.0026	0.0564	0.0000	0.0000
Diglycerol	0.4130	0.4130	0.0000	0.4329	0.0000
Triglycerol	0.0084	0.0084	0.0000	0.0088	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0122	0.0122	0.0000	0.0128	0.0000

Table S.2. Process streams for the maximum diglycerol production configuration (continuation).

Stream	22	23	24	25	26
Temperature (°C)	185.8	185.8	25.0	25.04	0.2116
Pressure (kPa)	3	3	3	101.3	101.3
Vapor fraction	1	1	0	0	0
Flow rate (kg/h)	1683	4.848×10^{-2}	1683	1683	0.1655
Enthalpy (kcal/kg)	-1462	-3098	-1759	-1759	-3804
Mass fractions					
Glycerol	1.0000	0.0000	1.0000	1.0000	0.0000
Argon	0.0000	0.0000	0.0000	0.0000	0.0000
Water	0.0000	0.9865	0.0000	0.0000	1.0000
Cesium bicarbonate	0.0000	0.0080	0.0000	0.0000	0.0000
Diglycerol	0.0000	0.0055	0.0000	0.0000	0.0000
Triglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000
Stream	**27**	**28**	**29**	**30**	**31**
Temperature (°C)	25	260.5	226.9	200	226.2
Pressure (kPa)	101.3	3	1	1	1
Vapor fraction	0	0	0.2414	0	1
Flow rate (kg/h)	1685	1403	1403	1403	1336
Enthalpy (kcal/kg)	-1761	-415.6	-415.6	-457.1	-340.7
Mass fractions					
Glycerol	0.9990	0.0001	0.0001	0.0001	0.0001
Argon	0.0000	0.0000	0.0000	0.0000	0.0000
Water	0.0010	0.0000	0.0000	0.0000	0.0000
Cesium bicarbonate	0.0000	0.0000	0.0000	0.0000	0.0000
Diglycerol	0.0000	0.9524	0.9524	0.9524	0.9998
Triglycerol	0.0000	0.0193	0.0193	0.0193	0.0001
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0281	0.0281	0.0281	0.0000
Stream	**32**	**33**	**34**	**35**	
Temperature (°C)	265.4	211.0	125.8	296.8	
Pressure (kPa)	1.0	0.005	0.005	0.005	
Vapor fraction	0	0.5165	1.0	0	
Flow rate (kg/h)	66.44	66.44	26.93	39.51	
Enthalpy (kcal/kg)	-410.5	-410.5	-393.2	-411.0	
Mass fractions					
Glycerol	0.0000	0.0000	0.0000	0.0000	
Argon	0.0000	0.0000	0.0000	0.0000	
Water	0.0000	0.0000	0.0000	0.0000	
Cesium bicarbonate	0.0000	0.0000	0.0000	0.0000	
Diglycerol	0.0001	0.0001	0.0001	0.0000	
Triglycerol	0.4056	0.4056	0.9999	0.0006	
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	
Larger oligomers	0.5944	0.5944	0.0000	0.9994	

Table S.3. Process streams for the maximum triglycerol production configuration.

Stream	Glycerol Inlet	Glycerol Recycle	Argon Inlet	Argon Recycle	Water
Temperature (°C)	25	25	25	25	25
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	0	0	1	1	0
Flow rate (kg/h)	1559	389.3	8.390 x	62.47	19.42
Enthalpy (kcal/kg)	-1761	-1761	-5.591	-5.589 x 10^{-2}	-3780
Mass fractions					
Glycerol	0.9990	0.9990	0.0000	0.0000	0.0000
Argon	0.0000	0.0000	1.0000	1.0000	0.0000
Water	0.0010	0.0010	0.0000	0.0000	1.0000
Cesium bicarbonate	0.0000	0.0000	0.0000	0.0000	0.0000
Diglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Triglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000
Stream	**Catalyst**	**Glycerol**	**Argon**	**Water + Catalyst**	**1**
Temperature (°C)	25	25	25	25	260
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	0	0	1	0	0
Flow rate (kg/h)	7.794	1948	62.56	27.22	1948
Enthalpy (kcal/kg)	-1005	-1761	-	-2985	-1601
Mass fractions					
Glycerol	0.0000	0.9990	0.0000	0.0000	0.9990
Argon	0.0000	0.0000	1.0000	0.0000	0.0000
Water	0.0000	0.0010	0.0000	0.7136	0.0010
Cesium bicarbonate	1.0000	0.0000	0.0000	0.2864	0.0000
Diglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Triglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000
Stream	**2**	**3**	**4**	**5**	**6**
Temperature (°C)	260	260	260	260	105
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	1	1	1	0	0
Flow rate (kg/h)	62.56	27.22	412.4	1625	260.0
Enthalpy (kcal/kg)	29.20	-2322	-1738	-619.0	-2102
Mass fractions					
Glycerol	0.0000	0.0000	0.3101	0.1605	0.4919
Argon	1.0000	0.0000	0.1514	0.0001	0.0000
Water	0.0000	0.7136	0.4046	0.0042	0.3124
Cesium bicarbonate	0.0000	0.2864	0.0182	0.0002	0.0124
Diglycerol	0.0000	0.0000	0.1156	0.8351	0.1833
Triglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000

Table S.3. Process streams for the maximum triglycerol production configuration (continuation).

Stream	7	8	9	10	11
Temperature (°C)	105	0	0	0	0
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	1	1	0	1	0
Flow rate (kg/h)	152.4	62.62	89.81	62.45	0.1735
Enthalpy (kcal/kg)	-1791	-11.68	-3671	-3.173	-3657
Mass fractions					
Glycerol	0.0002	0.0000	0.0003	0.0000	0.0000
Argon	0.4097	0.9972	0.0000	1.0000	0.0000
Water	0.5620	0.0026	0.9520	0.0000	0.9469
Cesium bicarbonate	0.0281	0.0001	0.0477	0.0000	0.0531
Diglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Triglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000
Stream	**12**	**13**	**14**	**15**	**16**
Temperature (°C)	25	212.2	254.1	254.1	254.1
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Vapor fraction	1	0.2155	1	0	0.3865
Flow rate (kg/h)	62.45	1885	195.4	1690	1885
Enthalpy (kcal/kg)	-5.589×10^{-2}	-823.5	-2220	-661.2	-822.8
Mass fractions					
Glycerol	0.0000	0.2062	0.3674	0.1876	0.2062
Argon	1.0000	0.0001	0.0006	0.0000	0.0001
Water	0.0000	0.0467	0.5352	0.0063	0.0612
Cesium bicarbonate	0.0000	0.0019	0.0164	0.0002	0.0019
Diglycerol	0.0000	0.7452	0.0703	0.4907	0.4471
Triglycerol	0.0000	0.0000	0.0102	0.1432	0.1294
Tetraglycerol	0.0000	0.0000	0.0000	0.0789	0.0705
Larger oligomers	0.0000	0.0000	0.0000	0.0934	0.0837
Stream	**17**	**18**	**19**	**20**	**21**
Temperature (°C)	203.1	165.0	53.12	207.4	185.4
Pressure (kPa)	3	3	3	3	3
Vapor fraction	0.6055	0.4240	1	0	1
Flow rate (kg/h)	1885	1885	118.9	1766	388.8
Enthalpy (kcal/kg)	-822.8	-874.5	-3110	-710.8	-1462
Mass fractions					
Glycerol	0.2062	0.2062	0.0005	0.2201	0.9998
Argon	0.0001	0.0001	0.0009	0.0000	0.0000
Water	0.0612	0.0612	0.9691	0.0000	0.0001
Cesium bicarbonate	0.0019	0.0019	0.0295	0.0000	0.0000
Diglycerol	0.4471	0.4471	0.0000	0.4772	0.0002
Triglycerol	0.1294	0.1294	0.0000	0.1381	0.0000
Tetraglycerol	0.0705	0.0705	0.0000	0.0752	0.0000
Larger oligomers	0.0837	0.0837	0.0000	0.0893	0.0000

Table S.3. Process streams for the maximum triglycerol production configuration (continuation).

Stream	22	23	24	25	26
Temperature (°C)	185.8	185.8	25.0	25.04	0.2116
Pressure (kPa)	3	3	3	101.3	101.3
Vapor fraction	1	0.7824	0	0	0
Flow rate (kg/h)	388.7	9.036×10^{-2}	388.7	388.7	0.3821
Enthalpy (kcal/kg)	-1462	-1043	-1759	-1759	-3804
Mass fractions					
Glycerol	1.0000	0.0000	1.0000	1.0000	0.0000
Argon	0.0000	0.0000	0.0000	0.0000	0.0000
Water	0.0000	0.2222	0.0000	0.0000	1.0000
Cesium bicarbonate	0.0000	0.0021	0.0000	0.0000	0.0000
Diglycerol	0.0000	0.7756	0.0000	0.0000	0.0000
Triglycerol	0.0000	0.0001	0.0000	0.0000	0.0000
Tetraglycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Larger oligomers	0.0000	0.0000	0.0000	0.0000	0.0000
Stream	**27**	**28**	**29**	**30**	**31**
Temperature (°C)	25	267	167.7	152.8	183.0
Pressure (kPa)	101.3	3	0.05	0.05	0.05
Vapor fraction	0	0	0.6990	1	0
Flow rate (kg/h)	389.1	1378	1378	843.0	534.6
Enthalpy (kcal/kg)	-1761	-410.7	-410.7	-380.1	-456.7
Mass fractions					
Glycerol	0.9990	0.0000	0.0000	0.0001	0.0000
Argon	0.0000	0.0000	0.0000	0.0000	0.0000
Water	0.0010	0.0000	0.0000	0.0000	0.0000
Cesium bicarbonate	0.0000	0.0000	0.0000	0.0000	0.0000
Diglycerol	0.0000	0.6118	0.6118	0.9998	0.0001
Triglycerol	0.0000	0.1771	0.1771	0.0001	0.4562
Tetraglycerol	0.0000	0.0965	0.0965	0.0000	0.2486
Larger oligomers	0.0000	0.1145	0.1145	0.0000	0.2952
Stream	**32**	**33**	**34**	**35**	**36**
Temperature (°C)	124.7	250	126.6	283.4	280.7
Pressure (kPa)	0.001	0.001	0.001	0.001	0.001
Vapor fraction	0	0.6392	1	0	1
Flow rate (kg/h)	534.6	534.6	243.9	290.6	132.9
Enthalpy (kcal/kg)	-456.7	-378.4	-392.9	-422.0	-337.9
Mass fractions					
Glycerol	0.0000	0.0000	0.0000	0.0000	0.0000
Argon	0.0000	0.0000	0.0000	0.0000	0.0000
Water	0.0000	0.0000	0.0000	0.0000	0.0000
Cesium bicarbonate	0.0000	0.0000	0.0000	0.0000	0.0000
Diglycerol	0.0001	0.0001	0.0001	0.0000	0.0000
Triglycerol	0.4562	0.4562	0.9997	0.0001	0.0001
Tetraglycerol	0.2486	0.2486	0.0001	0.4571	0.9997
Larger oligomers	0.2952	0.2952	0.0000	0.5429	0.0001

Table S.3. Process streams for the maximum triglycerol production configuration (continuation).

Stream	**37**
Temperature (°C)	322.3
Pressure (kPa)	0.001
Vapor fraction	0.0000
Flow rate (kg/h)	157.8
Enthalpy (kcal/kg)	-398.1
Mass fractions	
Glycerol	0.0000
Argon	0.0000
Water	0.0000
Cesium bicarbonate	0.0000
Diglycerol	0.0000
Triglycerol	0.0000
Tetraglycerol	0.0001
Larger oligomers	0.9999

S.5- The effects of vacuum distillation on the costs of the distillation columns

Vacuum distillation affects the costs of the columns in two ways: by adding an additional thickness to the column vessel, which contributes to its weight and, therefore, to its cost; and by the necessity to account for a specific device for vacuum generation.

According to Seider et al.,[1] the thickness of the columns can be calculated with the following equations:

$$t_s = t_v + t_c \quad \text{(S.3)}$$

$$t_v = 1.3 D_O \left(\frac{PL}{E_M D_O}\right)^{0.4} + t_{vc} \quad \text{(S.4)}$$

$$t_{vc} = L(0.18 D_i - 2.2) \times 10^{-5} - 0.19 \quad \text{(S.5)}$$

where t_s is the column shell thickness (according to the authors, it is sufficient for cost-estimation purposes to assume the thicknesses of the two heads to be equal to the shell thickness); t_v is the primary wall thickness of the vessel, which is a function of the design pressure P, in psi, the length-to-outside diameter ratio L/D_O, and the modulus of elasticity, E_M, in psi, which depends on temperature; t_{vc} is a correction in terms of length, L, and inside diameter, D_i; and t_c is a corrosion allowance of 1/8 in that must be added to t_v even for noncorrosive conditions.

Vacuum is generated with a device such as (multi)stage steam-jet ejectors, (multi)stage liquid-ring pumps and dry vacuum pumps. For the volume flow rates and pressures observed in the columns of this work, devices of the first type are recommended.[1] Then, their costs can be calculated with the following equation:

$$C_{vacuum} = F_{MS} \times 1{,}915 \times \left(\frac{Q}{P}\right)^{0.41} \qquad \text{(S.6)}$$

where Q is the suction volume flow rate in lb/h; P is the suction pressure, in torr; and F_{MS} is a multistage factor which is 1.8 for two stages (suction pressure limit of 15 torr or ~ 0.0200 bar) and 2.1 for three stages (suction pressure limit of 2 torr or ~ 0.0027 bar).[1]

With Equation S.6, the costs presented in Table S.4 were calculated for the vacuum apparatus associated to every column.

Table S.4. Participation of the vacuum apparatus in the cost of the distillation columns.

Maximum production of diglycerol					
	T-100	T-101	T-102	T-103	
Total cost [a]	176,008.45	688,637.28	2,363,354.79	404,505.43	
Vacuum apparatus	76,323.69	107,736.52	103,226.15	358,849.05	
Percentage [b]	17.79%				
Maximum production of triglycerol					
	T-100	T-101	T-102	T-103	T-104
Total cost [a]	151,295.19	240,445.79	4,041,126.21	1,874,337.77	2,713,839.98
Vacuum apparatus	61,164.54	85,702.19	483,861.14	1,632,362.99	1,271,312.46
Percentage [b]	39.18%				

[a] Including condenser and reboiler.
[b] Sum of the costs of all vacuum apparatuses divided by the sum of the total costs of all columns.

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