
**Supply chain optimization of integrated glycerol biorefinery: GlyThink
model development and application**

Supporting Information for publication

Table S1: Market demands for each product, corresponding main assumptions and respective references.

Products	Markets	Demand per market (10 ³ ton/year)	Assumptions	Refs
PHB	Germany	8.82×10 ³	Potential addressable market is as replacement of polypropylene (PP) and polyethylene (PE)	(1)(2)
	France	4.97×10 ³		
	Italy	3.37×10 ³		
	United Kingdom	2.64×10 ³		
	Spain	2.60×10 ³		
Ethanol	Germany	1.20×10 ⁶	Bioethanol used as biofuel	(3)
	UK	7.89×10 ²		
	France	6.71×10 ²		
	Spain	2.96×10 ²		
	Italy	2.84×10 ²		
Lactic acid	Germany	5.36×10 ³	Production of PLA, with an addressable market as replacement of polystyrene (PS), polypropylene (PP) and PET → this market represents 39% of the total market of lactic acid	(1) (2)(4)
	France	3.02×10 ³		
	Italy	2.05×10 ³		
	UK	1.60×10 ³		
	Spain	1.85×10 ³		
Succinic acid	UK	2.56×10 ²	Addressable markets are given by plasticizers, BDO, polyester polyols, alkyl resins, PBS and PBST	(2),(5,6)
	Spain	2.52×10 ²		
	Germany	8.54×10 ²		
	Italy	4.81×10 ²		
	France	3.26×10 ²		
1,3-propanediol	Germany	1.22×10 ³	For the production of PTT, which is a biodegradable replacement for PET	(1)(2)
	France	6.87×10 ²		
	Italy	4.66×10 ²		
	UK	3.65×10 ²		
	Spain	3.60×10 ²		
1,2-propanediol (propylene glycol)	Germany	4.90×10 ²	Top-5 major propylene glycol producers	(7)
	Netherlands	80		
	France	80		
	Spain	95		
	Belgium	50		
H₂	Germany	2.44×10 ⁶	16% of the world demand corresponds to western Europe, top-5 distribution based on the GDP of the individual countries	(8,9)
	France	1.78×10 ⁶		
	Netherlands	5.54×10 ⁵		
	Belgium	3.36×10 ⁵		
	Austria	2.77×10 ⁵		
Acrolein	Bulgaria	9.15×10 ²	Addressable market is acrylic acid and the demand was given in total for eastern and western Europe, the top-5 distribution was given based on the GDP of the individual countries	(8,10,11)
	Germany	6.35×10 ²		
	Belgium	3.20×10 ²		
	France	2.75×10 ²		
	Czech Republic	55		
Propionic acid	Germany	67.5	Propionic acid demand in the world, where 16% is for Europe. GDP was used to find the top-5 consumers	(8,12)
	France	49.3		
	Netherlands	15		
	Belgium	92.7		
	Austria	7.65		
n-Butanol	Germany	2.19×10 ²	European demand of n-butanol	(13–15)
	UK	1.58×10 ²		
	France	1.65×10 ²		
	Italy	35.3		
	Spain	82		
Isobutanol	Belgium	94.7	Isobutanol is used as a precursor of terephthalic acid, which is a precursor of PE. The same distribution as the one for plastics in Europe	(16,17)
	Portugal	49.4		
	Spain	49.4		
	Poland	42.4		
	UK	35.3		

Epichlorohydrin	Germany	1.58×10 ²	Addressable market is the production of epoxy resins. For this, bisphenol A (BPA) is used along with epichlorohydrin. 30% of the consumption of BPA is for the production of epoxy resins. World demand of BPA and the respective percentage for Europe. Top-5 consumers of BPA assumed to be the same for epichlorohydrin.	(18–20)
	Netherlands	1.42×10 ²		
	Belgium	96.7		
	Spain	86.8		
	Italy	42.7		

Table S2: Matrix of distances between the plant site and the markets.

(km)	Germany	France	Netherlands	Spain	Italy
Germany	383.5	1032.7	467.3	2058.7	1376.3
France	1032.7	529.5	853.9	1001.6	1298
Italy	1376.3	1298	1621.9	1974.1	410
UK	1471.5	1428	1017.3	2311.3	2472.5
Spain	2058.7	1001.6	1753.9	471	1974.1
The Netherlands	467.3	853.9	131.4	1753.9	1621.9
Belgium	543.2	658	224.7	1549.7	1467.2
Austria	685.6	1308.4	1024.6	2242	933.9
Bulgaria	1972.8	2390.9	2412.9	3270.6	1962.5
Czech Republic	529.4	1313	932.4	2416.9	1371.1
Poland	755.9	1710	1023.5	2716.8	3053.9
Portugal	2397.3	1340.2	2092.6	477.8	2389.5

Table S3: Product prices, reference capacity and reference purchased capital investment.

Product	Reference capacity (ton/year)	Purchased Capital Cost (MM\$)
Succinic acid (SA)	10200	11.217 (21)
1,3-propanediol (13pdo)	5500	5.347 (21)
Propionic acid (PA)	6796	4.747 (21)
Polyhydroxybutyrate (PHB)	3600	15.020 (21)
1,2-propanediol (12pdo)	7740	4.713 (21)
Lactic acid (LA)	7931	4.929 (21)
Isobutanol (Isob)	7300	6.705 (21)
Hydrogen (H ₂)	659	5.551 (21)
n-Butanol (BuOH)	3000	5.202 (21)
Ethanol (EtOH)	5211	8.227 (21)
Acrolein (Acro)	4870	4.927 (21)
Epichlorohydrin (epi)	100000 (22)	166 (23)

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