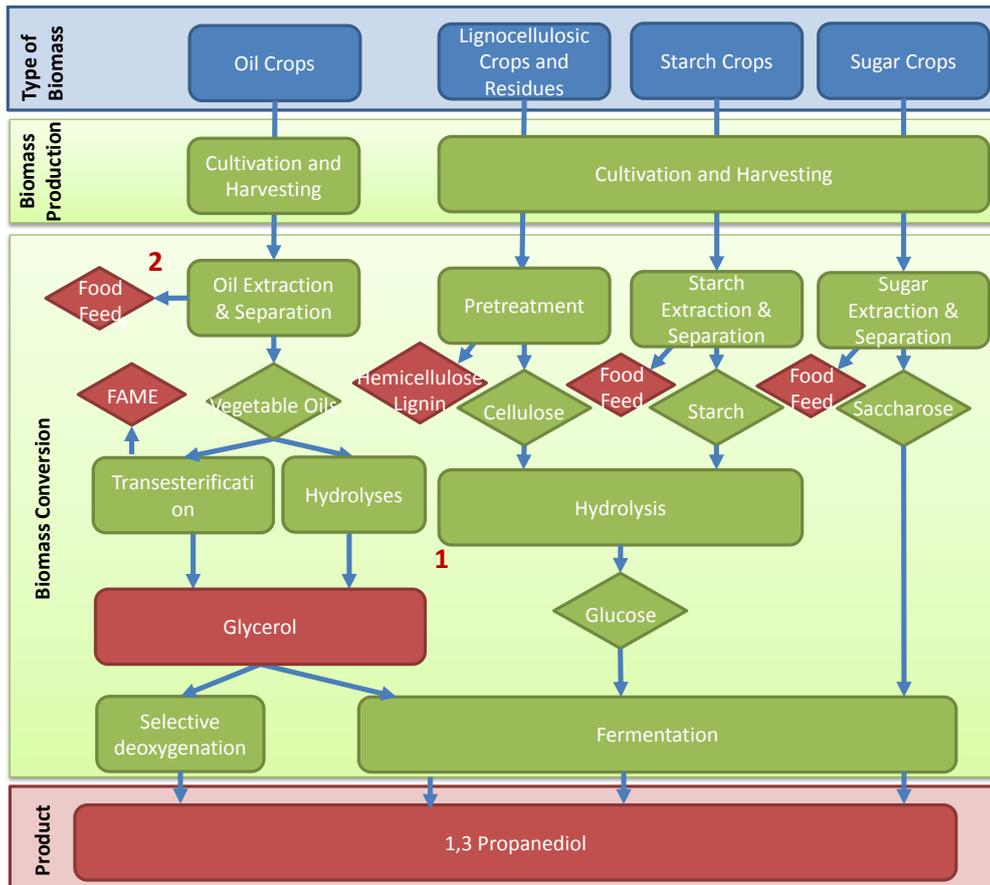


ENVIRONMENTAL FACTSHEET: 1,3-PROPANEDIOL

PRODUCT INFORMATION

1,3-propanediol (1,3-PDO) is a bifunctional organic compound with chemical formula $\text{OHCH}_2\text{CH}_2\text{CH}_2\text{OH}$. 1,3-PDO is a building block chemical that can be used in the preparation of the bio-based polymer polytrimethylene and in the production of adhesives, paints, resins and coatings.



1,3-PDO can be chemically synthesised from fossil based compounds such as propenal or ethylene oxide. The majority of 1,3-PDO production is thought hydroformylation of ethylene oxide.

The bio-based pathways include fermentation of glycerol (see glycerol factsheet¹) or fermentation of sugars. Therefore, 1,3-PDO can be produced from a range of biomass feedstock - sugar or starch crops, lignocellulosic materials, oils crops and residues. The maturity of various 1,3-PDO production technologies is summarised in Figure 2. The use of lignocellulosic materials appears the least advanced production system. The sugar fermentation path is commercial available using genetically modified bacteria *E. Coli*. Glycerol is a by-product of biodiesel

Figure 1. 1,3-PDO production chains *FAME-Fatty acid methyl esters (biodiesel)

(see biodiesel via transesterification factsheet²) production and can be fermented to produce 1,3-PDO using bacteria such as *Klebsiella pneumonia*, *Clostridium butyricum* and *Citobacter freundii*, [1]. However, the use of mix bacterial cultures has also been proposed.

1,3-PDO can be chemically synthesised also by selective deoxygenation (or selective reduction) of glycerol using organometallic catalysts.

After fermentation the commercial available process for separation of 1,3-PDO from the fermentation broth consists of micro- and ultra-filtration, ion exchange separation, evaporation and distillation.

Technology Readiness Levels

		1,3-PDO production from fermentation of glycerol using pure bacterial cultures							1,3-PDO production from fermentation of glucose using modified <i>E. Coli</i>
		1,3-PDO production from fermentation of sugars produced from lignocellulosic material							
		1,3-PDO production from fermentation of glycerol using mix bacterial cultures							
		1,3-PDO production from glycerol through selective deoxygenation							
1	2	3	4	5	6	7	8	9	
Basic research	Technology formulation	Applied research	Small scale prototype	Large scale prototype	Prototype system	Demonstration system	Completed commercial system	Full commercial application	

Figure 2. Technology readiness levels for 1,3-PDO production

SWOT (Strengths, Weaknesses, Opportunities, Threats)

<p>S1. Biobased production pathway already at full commercial scale.</p> <p>S2. 1,3-PDO has a high variety of applications which results in increasing demand of this product.</p>	<p>W1. The glycerol production pathway has low yields and it is inhibited by substrate and product.</p> <p>W2. Difficult recovery of 1,3-PDO from fermentation broth.</p>
<p>O1. The increased availability of glycerol may boost the development of the glycerol fermentation pathway.</p>	<p>T1. Biomass availability for the biobased production pathway.</p> <p>T2. Competition with food and feed.</p>

ENVIRONMENTAL DATA AND INFORMATION

The environmental performance of 1,3-PDO is summarised in Table 1, based on the available relevant LCA data for 1,3-PDO production, using different raw materials (corn, sugar cane, corn stover and rapeseed) through: 1. aerobic fermentation of sugars, or 2. anaerobic fermentation of glycerol and 3. purification through evaporation, crystallisation and distillation.

Most of the values presented refer to cradle to gate (see Figure 3) LCA approach. When the cradle to grave approach is considered [1], the climate change results are found to increase up to 80% depending on the specific end-of-life scenario.

The most widely reported impact categories are climate change, land use, primary energy and non-renewable energy use. Few or no results were found for the remaining impact categories of the environmental sustainability assessment methodology developed in the context of this project (see explanatory document).

System boundaries of the environmental assessment

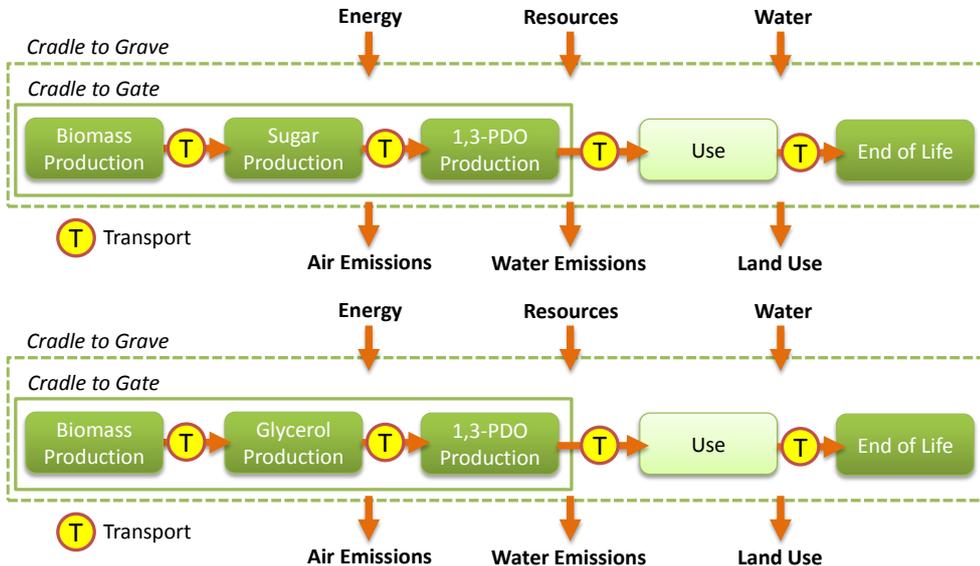


Figure 3. LCA system boundaries for 1,3-PDO production and end-of-life

1. Cradle to gate: includes the resources extraction (energy, materials and water), transport and the production steps until the gate of the 1,3-PDO factory.

2. Cradle to grave: additionally to the cradle to gate activities, this system includes the transport and distribution of the product, the use of 1,3-PDO and its end-of-life.

Environmental assessment: settings & impacts

Table 1. LCA results for one kg of 1,3-PDO in a cradle to gate system				
Raw material input (feedstock)	Corn	Sugar Cane	Corn stover	Rapeseed
Allocation/substitution	A(\$-m), S	A(\$-m), S	A(\$-m), S	A(\$-m), S
Geographical coverage	EU and US	Brazil	EU	EU
References	[2,3]	[2]	[2]	[2]
Impact categories from Environmental Sustainability Assessment methodology				
Climate change (kgCO ₂ eq)	(0.5-2.8)	(-1.7-(-)0.4) ¹	(-0.8-0.4) ²	(1.7-1.8) ⁴
Freshwater eutrophication (kgPO ₄ eq)	4.5E ⁻³ [3]	N.A	N.A	N.A
Additional impact categories				
Freshwater ecotoxicity (kg 1,4-DBeq)	1.26E ⁻⁷ [3]	N.A	N.A	N.A
Human toxicity – no cancer effects (kg 1,4-DBeq)	1.8E ⁻² [3]	N.A	N.A	N.A
Photochemical ozone formation (kg C ₂ H ₄ eq)	1.7E ⁻³ [3]	N.A	N.A	N.A
Acidification (kg SO ₂ eq)	4.5E ⁻² [3]	N.A	N.A	N.A
Marine ecotoxicity (kg 1,4-DBeq)	3.9E ⁻⁴ [3]	N.A	N.A	N.A
Terrestrial ecotoxicity (kg 1,4-DBeq)	8.1E ⁻⁷ [3]	N.A	N.A	N.A
Land use (m ²)	(2.7-3.1) [2]	(2.8-3.2)	(1.1-1.3) ³	(4.2-5.3) ⁴
Primary energy (MJ)	(79.7-95.2) [2]	(93.0-108.6)	(83.0-98.5)	(96.8-105.5) ⁴
Non-renewable energy (MJ)	(37.6-54.6)	(-8.6-14.5) ¹	(11.9-32.3) ²	(62.8-63.5) ⁴

Note: N.A. not available. A=Allocation (\$-economic; E-energy; m-mass). S=Substitution. SE=System expansion.

The normalisations presented in Figure 4 were performed using the normalisation factors provided by the JRC methodology [4] and the ReCiPe normalisation factors (see explanatory document).

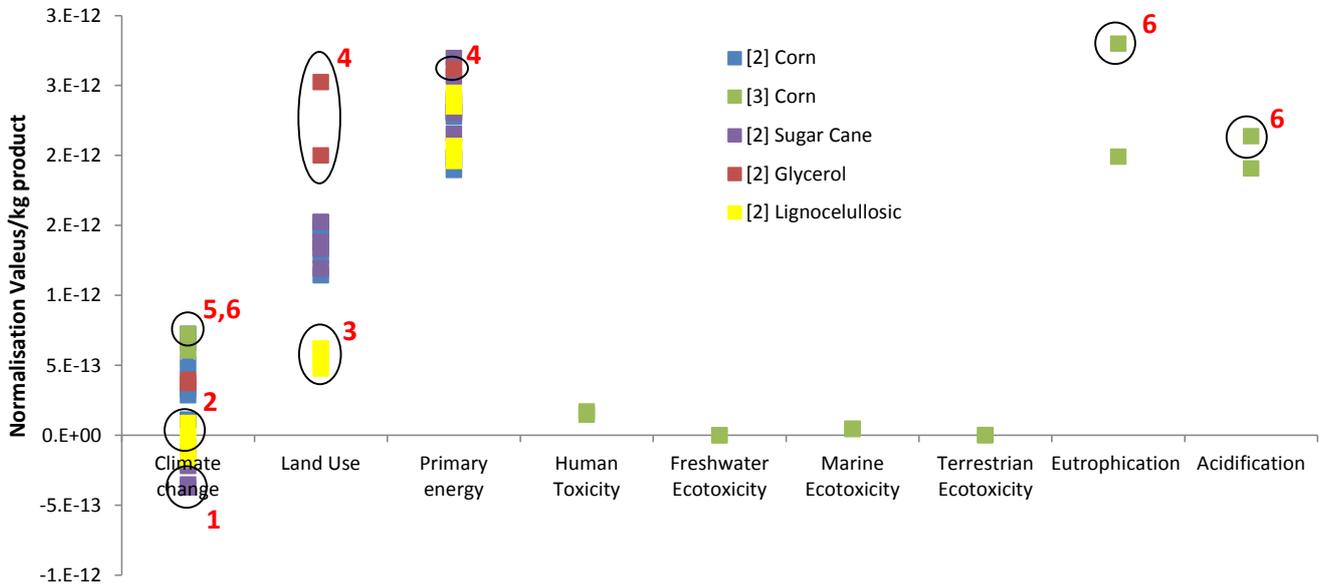


Figure 4. Environmental performance expressed as normalised impact categories

Comments and interpretation of environmental performance (Table 1 and Figure 4):

1. The lowest values found for climate change and non-renewable energy demand were obtained for the production of 1,3-PDO from sugar cane, owing to the high productivity yields of sugar and the credits assigned to the process [2] for the energy surplus, generated from bagasse burn;
2. Reference [2] considers the burning of lignin-rich waste [obtained in the pretreatment (hydrolyses) (see bioalcohols via fermentation factsheet) of corn stover] to produce power and heat. This results in decreased impacts in non-renewable energy demand and climate change categories;
3. The land requirements for 1,3-PDO production using corn stover are lower compared to corn, sugar cane and glycerol. This is mainly due to the economic allocation applied [2], which assigns a lower value to corn stover than corn kernels;
4. The environmental impacts of producing 1,3-PDO from glycerol are usually higher compared to the other feedstock pathways, because glycerol earns lower fermentation yields and requires higher land use per kg of end-product;
5. The highest values found for climate change impacts were obtained from studies which took into account cradle to grave boundaries [2], from which it can be concluded that the end-of-life phases are environmentally significant;
6. In reference [3] higher values were found when no allocation was considered (compared with the use of mass allocation), which fact indicates the influence of allocation on the environmental performance. However, environmental impacts decrease when substitution is applied, as in this case the system is credited for the production of by-products (see comments 1 and 2).

REFERENCES / FURTHER INFORMATION

[1] Kraus, 2008. Clean 36: 648 – 651.
 [2] BREW Project - Medium and long-term opportunities and risks of the biotechnological production of bulk chemicals from renewable resources. <http://brew.geo.uu.nl/>
 [3] Urban et al., 2009. Ind. Eng. Chem. Res. 48: 8068–8082.
 [4] Benini et al., Normalisation method and data for Environmental Footprints, JRC Technical Report, Draft v.2014.

FP7 Project REFERENCES in CORDIS www.cordis.europa.eu
BIO-TIC
4FCrops