Life Cycle Analysis Overview - Zemea® Propanediol

Introduction

DuPont Tate & Lyle Bio Products (DT&L) is a 50/50 joint venture between DuPont of Wilmington, Delaware and Tate & Lyle of London that was formed to develop and commercialize 1,3 propanediol made from renewable resources. In November 2006, construction was completed on a world scale aerobic fermentation facility in Loudon, Tennessee. This facility utilizes a proprietary fermentation process to convert glucose into Zemea® propanediol.

Zemea® propanediol, also known as Bio-PDO™, is chemically identical to pure petroleum derived 1,3-propanediol with identical attributes and functionalities. All carbon in Bio-PDO™ is bio-based.

A cradle-to-gate life cycle assessment (LCA) for Bio-PDO™ based on ISO 14040 guidelines was completed on Zemea® propanediol using plant data for Bio-PDO™, updating a 2006 LCA which had used design data. Like the original LCA, this study was commissioned and performed by DuPont engineers in accordance with ISO standard 14040 and peer-reviewed by a 3rd-party review panel. The following outline includes frequently asked questions that provide additional information on the production, processes, methodology, and results for the Zemea® propanediol.

Production

The manufacturing plant in Loudon, TN is located adjacent to Tate & Lyle's corn wet mill that supplies the glucose from corn starch to DT&L. The glucose is introduced to the biocatalyst and converted to 1,3 propanediol through the fermentation process using a patented microorganism under exact temperatures and conditions. The 1,3 propanediol is refined to a final purity of 99.7% by deactivating and removing the microorganism, water and other byproducts.

Methodology – What methodology did DuPont use in the LCA for Zemea® Propanediol?

General

In accordance to ISO 14040 all significant raw materials, utilities and process outputs including emissions were considered as a part of the life cycle inventory from the growing of corn grain through the production of Bio-PDO™. At a minimum, materials contributing more than 1% of the mass, and materials suspected or known to contribute significantly to the impact metrics of interest in this study were included. Site and region-specific energy and electricity information was used in the study. The ecoinvent version 3.1 database was used for most background models, including energy and electricity supply. Details on the modelling of the foreground models for corn grain, the corn wet mill, Bio-PDO™, and some key energy models are detailed below. The cradle-to-gate greenhouse gas emissions include a credit for bio-based carbon sequestered in the product.

Multiple sensitivity and scenario analyses were performed as part of the peer-reviewed LCA, including corn wet mill allocation scenarios, regional corn grain production, end-of-life modelling, among others.

The results represent data from 2016 and incorporate a new natural gas combined heat and power unit at the Loudon corn wet mill facility.

Functional Unit

The functional unit for this cradle-to-gate LCA is 1-kg of product. In product applications comparing different materials, a functional basis rather than a simple mass basis should be used. This is a known limitation of the study, but appropriate in the absence of a specific application.

Impact Categories

Four key impact metrics were identified for this study as follows:

- *Non-renewable Energy Consumption: Cumulative Energy Demand (CED) v. 1.09. Both fossil fuel and nuclear fuel Impacts are included [CED 2007]*
- *IPCC - Climate Change Potential 4th Assessment report (100 yr) [IPCC 2007]*
- *Required Farmland: Agricultural Land Occupation – ReCiPe Midpoint (H) v1.12 [ReCiPe 2009]; Excludes all forest related flows.*
- *Consumptive Water Use: Quantis Water Database [Quantis 2012]*

Other metrics were evaluated as part of the peer-reviewed LCA, but are not deemed to be as critical as the key metrics identified above.

The above impact categories represent impact potentials and do not predict actual impacts, the exceeding of thresholds, safety margins, or risks. Value choices are made in this study with respect to the selection of four key impact categories: NREU, CCP, land use, and water use.

<u>Inventory Analysis – What unit processes are modeled in the LCA?</u>

Corn Grain Production

Multiple corn LCA models in the literature were evaluated. The model available in ecoinvent database version 3.1, default (EI3.1) for U.S. corn grain was chosen as the basis for this study with several modifications, including updates for yield, fertilizer and agrochemical use rates, irrigation needs, and corrections to energy use for both drying and irrigation [ecoinvent 2016]. More specifically, yield is based on NASS data from 2010-2014 [NASS 2016], irrigation requirements are based on US average NASS statistics for 2013, and grain drying requirements are calculated from an estimated initial moisture content at harvest of 20 wt.% down to a final moisture content of 15 wt.%. The EI3.1 US corn model assumed 38% initial moisture which is well above combine harvested corn moisture [Nielson 2013]. Drying from 38% to 20% occurs naturally in the field.

Field N_2O emissions are calculated based on yield and fertilizer inputs using IPCC methodology with crop and region-specific values. The N_2O-N emission rate per inorganic nitrogen fertilizer applied is 1% direct N_2O-N plus 0.92 wt.% indirect N_2O-N emissions [IPCC 2013].

Corn Wet Mill

The input data for the corn wet mill (CWM) model were provided by Tate & Lyle and are based on the feedstock production for the 100 million pounds per year facility at Loudon, TN in 2004 [Tate & Lyle 2005]. Updates were not provided as the facility noted no significant changes as of 2015. However, in late 2016, natural gas combined heat and power (CHP) units were installed to provide the electricity for the corn wet mill and the steam for both the corn wet mill and the Bio-PDO™ facility. Energy use rates at the mill were not changed, but the burdens for the energy production are reduced based on the fuel source and improved efficiency of the CHP units.

The ISO 14040 standard recommends applying system expansion to avoid allocation where possible. System expansion, to account for the corn wet mill co-products, corn gluten meal (CGM), corn gluten feed (CGF), and corn germ meal, is incorporated by modeling them as displacing corn grain production based on their economic value. This methodology follows the methodology used in the Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) Model developed by Argonne National labs. Per GREET, 1-kg bone dry CGF is equivalent to 1-kg corn grain, while 1-kg bone dry CGM is equivalent to 1.529-kg corn grain [GREET 2015]. The corn germ meal is assumed equivalent to corn gluten feed since it is often sold as a mixture with CGF. Corn oil is assumed to displace the production of soybean oil, where soybean oil burdens per ecoinvent v3.1 models are used. Ecoinvent models use economic allocation for the soybean mill co-products. The impacts from the energy required to convert corn germ to corn germ meal and corn oil after it leaves the Loudon facility are subtracted from the credits provided for these co-products since they are not included in the Loudon CWM dataset. This energy is estimated using the Agri-footprint database unit process data for these process steps within a corn wet mill [Blonk 2015a, 2015b].

DuPont Tate & Lyle Facility (Bio-PDO™)

Bio-PDO™ production is based on 2015 plant operations for the Loudon, TN plant [Tate & Lyle 2005]. Steam supply is modeled assuming production via the new natural gas combined heat and power units. Electricity for the Bio-PDO™ facility is modelled from the U.S. SERC electricity grid. The production of the bacteria that produces the bio-based propanediol is included in the process model. A minor organic waste co-product of the Bio-PDO™ process is combined with the corn gluten feed from the CWM. This stream is modelled as CGF, displacing corn grain.

Energy models – How was the energy modeled?

Ideally, database energy, cogeneration, and electricity models available in SimaPro could be used throughout for this study. There are models in ecoinvent version 3.1 for heat, cogen, and regional electricity;however, the heat models are not US region specific and have an error in using higher heat value input flows, but lower heat value boiler efficiencies. Cogeneration models are also not available specifically for US regions and use economic allocation for steam and electricity co-production. Fuel specific electricity power generation models are available in ecoinvent for the US regions of interest and are used as the template for heat generation using typical heat and cogen fuel efficiencies as detailed below. While the technology is not specific to heat generation, the models developed do use regional fuel production data and the resulting impacts are higher than the ecoinvent heat models due to the heating value error.

The model, 'Electricity, high voltage {SERC}| electricity production, natural gas, at conventional power plant | Alloc Def, U' has emissions associated with the input of a specific quantity of natural gas associated with the production of 1 kWh electricity. This model is adjusted to be relevant for heat from natural gas by using the same emissions per cubic meter of natural gas supplied, and calculating a heat output based on a lower heating value (LHV) efficiency of 95.24% per ecoinvent 3.1, a LHV to higher heating value (HHV) ratio of 0.902 per GREET, and a HHV for natural gas of 38.3 MJ/m^3 based on the Cumulative Energy Demand (CED) impact assessment method [ecoinvent 2016, CED 2007].

The model, 'Electricity, high voltage {SERC}| electricity production, hard coal, at conventional power plant | Alloc Def, U' has emissions associated with the input of a specific quantity of coal associated with the production of 1 kWh electricity. This model is adjusted to be relevant for heat from coal by adjusting the output to MJ heat from coal on a LHV basis by using the same emissions per kg coal supplied, and calculating a heat output based on a HHV efficiency of 80% per ecoinvent 3.1, a regional adjustment factor for coal heat value of 1.321 per ecoinvent 3.1, and a general higher heat value for hard coal of 19.1 MJ/kg based on the CED impact assessment method used in ecoinvent [ecoinvent 2016, CED 2007].

The, 'Electricity, high voltage {SERC}| electricity production, natural gas, at conventional power plant | Alloc Def, U' model is adjusted to be relevant for heat and electricity generation based on the specific information for the new turbines installed at the Loudon corn wet mill site. The turbines are noted to have a heat rate of 9.882 MJ LHV per cubic meter of natural gas per kWh and an overall (steam plus electricity) LHV efficiency of 93.5%. For every kilowatt hour of electricity generated, 5.64 MJ steam are generated. Impacts are allocated between the steam and electricity based on conventional efficiencies per the World Business Council on Sustainable Development (WBCSD) recommendation [WBCSD 2006]. Conventional NG steam generation is noted to have a LHV efficiency of 95.24% per ecoinvent [ecoinvent 2016]. The installed turbines have a standard electricity generation LHV efficiency of 36.4% [Siemens 2009]. The LHV to HHV ratio is 0.902 per GREET and the HHV for natural gas is 38.3 MJ/m^3 per the CED impact assessment method used. At these efficiencies and production rates, 62.6% of the impacts of natural gas production and combustion are assigned to electricity generation and 37.4% to steam generation.

Transportation – Was transportation included in the LCA data?

Transportation burdens of raw materials throughout the supply chain are included in the evaluation, including transport of corn grain to Loudon, TN.

Benchmark Materials – How were the impacts for the benchmark materials calculated?

Two commercially viable benchmarks are identified for Bio-PDO™, including its isomer, propylene glycol, and 1,4-butanediol. Propylene glycol (PG) is produced exclusively through the hydrolysis of propylene oxide [Martin-Dow]. However, the propylene oxide (PO) production route has several technology options and the world supply is shifting towards newer technology. Six variations for modelling PO were evaluated in the peer-reviewed study. This report shares the results using the ecoinvent version 3.1 data for European production. A US LCI model modified to use ecoinvent 3.1 background processes results in 9% lower NREU and 14% lower GHG emissions. Results for propylene glycol are likely bounded by these two models. The ecoinvent model overestimates impacts due to its exclusive use of the chlorohydrin route for PO production, while the US LCI model likely underestimates impacts due to the use of mass allocation for co-products MTBE and styrene monomer.

The production of 1,4-butanediol (BDO) in the US is mainly via the Reppe process, involving the raw feeds of acetylene, formaldehyde, and hydrogen [Kumamoto 2016]. An ecoinvent model for BDO using the Reppe process is available based on a European supply chain. A US version of this model was developed by adjusting energy and natural gas feedstock supply to regional models consistent with US production. This required changes to the BDO unit process, as well as upstream processes for formaldehyde, methanol, acetylene, and oxygen production. This BDO-US model provides a representative model for comparing with US produced Bio-PDO™.

Petroleum-based PDO, a benchmark in the original LCA, is no longer commercially available. However, updated life cycle impact results for petroleum-based PDO production using ecoinvent version 3.1 background models is also included for comparison to Bio-PDO™ should it return to the market.

Results

Table 1 identifies the results for the four key impact metrics for Zemea® Propanediol and the three identified benchmark materials, propylene glycol, 1,4-butanediol, and petroleum-based 1,3-propanediol. All materials are evaluated on a 1-kg basis.

Table 1: Key Environmental Metrics for Zemea® Propanediol and benchmark materials per kg

Impact Category	Units (per kg)	Zemea® Propanediol	Petroleum-based 1,3-propanediol	Propylene Glycol	1,4-Butanediol
Non-Renewable Energy Use	MJ	56.1	108.8	95	103.8
Climate Change Potential	kg CO_2 eq	2.51	4.7	4.25	4.77
Water Use	liters	117	Not calc.	19.5	55.1
Agricultural Land Use	m^2	2.01	0	0	0

Water use for Zemea® Propanediol is dominated by irrigation needs for average U.S. corn grain. Water use for the benchmark materials is difficult to compare due to potential differences in the water use assumptions and definitions used in the US LCI and ecoinvent models used for this study. Land use is specific to agricultural land use. Any land use associated with wood-based fuels is excluded. Bio-based fuels could be used for any of these materials, resulting in a trade-off of reductions in NREU and CCP in exchange for increased land use.

Figures 1a and 1b show the climate change potential and non-renewable energy use for Zemea® Propanediol and the benchmark materials.

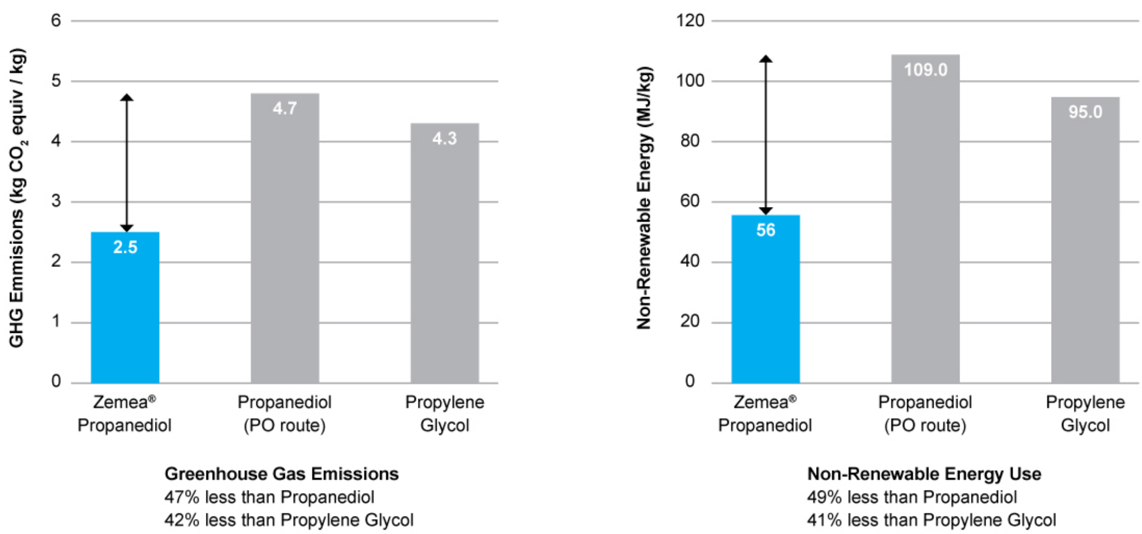

Figure 1a and 1b: Cradle-to-Gate Non-renewable Energy Use (NREU) and Climate Change Potential (CCP) for Zemea® propanediol and several benchmark materials on a 1-kg basis

The peer reviewed report from which this summary is based explored multiple corn grain models, allocation assumptions, and regional impacts of corn grain production. It also evaluated multiple literature results for benchmark materials. In general, it discussed at length, the various assumptions and assertions made in the study while providing the reviewers with the data required to validate the calculations and declare the study to have been performed in accordance with the ISO 14040 guidelines.

The 3rd-party peer review panel was as follows:

Critical Review Team Leader:

Professor Jay S. Golden, East Carolina University

Critical Review Team Members:

Professor Richard Venditti, North Carolina State University
Professor Roland Geyer, University of California Santa Barbara
Barruch Ben-Zekry, Director Sustainable Products & Materials, VF Corporation

A list of reviewer comments and DuPont responses as well as the review panel report can be made available upon request.

It must be noted that the panel review has the following limitations per ISO:

- A critical review can neither verify nor validate the goals that are chosen for an LCA, nor the ways the results are used.
- In no way does the review imply endorsement of any comparative assertion that is based on the LCA by members of the review panel.

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Krieger 2017	Krieger, T., et.al., “Life Cycle Assessment Update for Bio-PDOTM and Sorona® Polymer,” DuPont peer-reviewed internal study, September 2017.
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ZEMEA™ PROPANEDIOL
ENVIRONMENTAL DATA SHEET

BACKGROUND INFORMATION

	Our Product	Petroleum-Based Product	Substitute Product	Substitute Product
Product Name	Zemea® renewably sourced propanediol	Petroleum-based 1,3-propanediol	Propylene glycol	1,4 Butanediol
Chemical Name	1,3 propanediol	1,3 propanediol	1,2 propanediol	1,4 butanediol
Major Uses	Functional fluids, polymer intermediates	Polymer intermediates (Not currently commercial)	Personal care, functional fluids, coatings	Functional fluids, polymer intermediates
DuPont manufacturing Location	DuPont Tate & Lyle Bio Products Company, LLC, Loudon, TN	N/A	N/A	N/A

CRADLE-TO-GATE ENVIRONMENTAL METRICS

Greenhouse Gas Emissions kg CO_2 eq / kg	**2.5** [1,2]	**4.7** [1,3]	**4.3** [1,4]	**4.8** [1,4]
Non-Renewable Energy Use MJ / kg	**56** [1,5]	**109** [1,5]	**95** [1,4,5]	**104** [1,4,5]
Water Consumption liters / kg	**117** [1,6]	n/a [1,7]	**20** [1,6]	**55** [1,6]
Agricultural Land Use m^2 / kg	**2.0** [1,8]	n/a	n/a	n/a

PRODUCT PROPERTIES

Renewable Content % by wt.	**100%**	**0%**	**0%**	**0%**
Bio-based Carbon Content[9] % by wt.	**100%**	**0%**	**0%**	**0%**
Biodegradability[10]	**Yes**	**Yes**	**Yes**	**Yes**
Compostability[11]	n/a	n/a	n/a	n/a

Other Information

DuPont™ Renewably Sourced™ Materials contain a minimum of 20% renewably sourced ingredient by weight.

REFERENCES

[1] Krieger, T., et.al, "Life Cycle Assessment Update for Bio-PDO™ and Sorona® Polymer; Peer-reviewed LCA
[2] Includes bio-based carbon sequestered in product
[3] Assumes Degussa propylene oxide route; not currently commercial
[4] Ecoinvent v3.1 default allocation, modified for US fuel supply;
[5] Based on higher heating values (HHV)
[6] Following water impact methodology in Vionnet S., et. al., "Quantis Water Database – Technical Report," Quantis Water Database Consortium, 2012.
[7] Data on water use was unavailable. Not currently commercial
[8] Land use impacts per ReCiPe midpoint model, http://www.lcia-recipe.net.
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[10] ASTM Standard E1720 Standard Test Method for Determining Ready, Ultimate, Biodegradability of Organic Chemicals in a Sealed Vessel CO2 Production Test
[11] ASTM Standard D6400 Standard Specification for Compostable Plastic

For additional information or samples:

DuPont Tate & Lyle Bio Products
Customer Service

198 Blair Bend Drive

Loudon, TN 37774

Tel: +1-866-404-7933

www.duponttateandlyle.com