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Life Cycle Assessment (LCA) of Naturally-Sourced and Petroleum-Based Glycols Commonly Used in Personal Care Products

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abstract

Glycols, including 1,3-butylene glycol (1,3-BG), play an important role in the development of personal care products, including creams, sunscreens, shampoos, body washes and more. As concern about petroleum-based ingredients continues to grow, consumers have become increasingly concerned about the ingredient sources and manufacturing processes involved with making their products, including consideration of an ingredient's lifecycle impact and overall natural and sustainability attributes. To address these concerns, Genomatica has conducted a systematic study, called a life cycle assessment (LCA), on the environmental impact of the production process they've developed for their naturally-sourced, bio-based 1,3-BG (known as Brontide™), as compared with a petroleum-based alternative. The results show that conventional 1,3-BG production processes starting from petroleum-based feedstocks have a significantly higher global warming potential (103% greater) and energy demand from non-renewable resources (85% greater) relative to the bio-based process used to make Brontide from renewable plant-based feedstocks. The results of this study will help personal care and cosmetics formulators choose ingredients that have a reduced environmental impact while also addressing their customers' increasing desire for more natural products, helping manufacturers work toward a more sustainable future.

Traditional 1,3-Butylene Glycol Production and a Natural Alternative

1,3-BG is a four-carbon organic intermediate used in personal care and cosmetics products. It functions as a humectant, solvent and emollient, giving it many applications in skin care, hair care and as a solvent for high-purity botanical extracts.

Traditionally, 1,3-BG has been produced by oxidizing ethylene, a petrochemical, using palladium chloride and cupric chloride catalysis to synthesize acetaldehyde. Through a production process that generally includes condensation, hydrogenation and removal of impurities via polishing and distillation, cosmetic grade 1,3-BG is made. Distinct from the factors covered in the LCA, many users of 1,3-BG have concerns about a process that involves acetaldehyde, which is a mutagen and Group 1 carcinogen.

Genomatica has developed an alternative process, called GENO BG™, for the production of cosmetic-grade 1,3-BG. The resulting product of this process is Brontide, a naturally-sourced, sustainably-produced butylene glycol that delivers superior quality and product safety. Production occurs through fermentation of plant-derived dextrose using an engineered strain of *E. coli* to produce crude 1,3-BG (**Fig. 1**). High-purity Brontide is then produced through additional distillation and purification steps.

What follows is a summary of a complete, end-to-end LCA study of the process used to make Brontide and the process used to make petroleum-based 1,3-BG. An LCA is a well-defined and well-established method for assessing the environmental impact of each step in the production of a product, from raw material extraction through disposal. Assessing these two

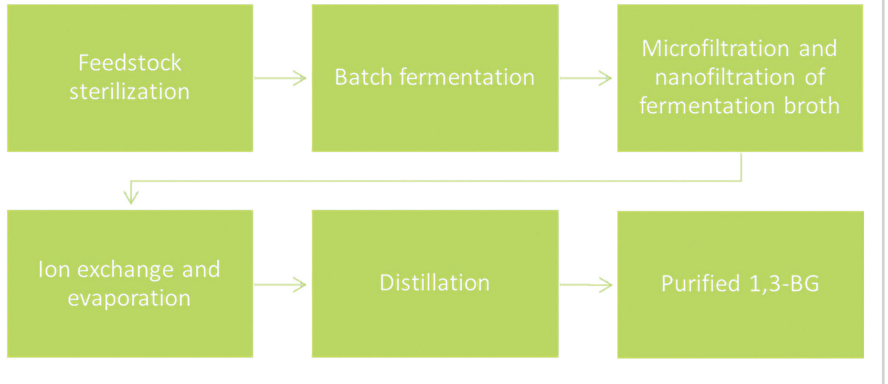

Fig. 1 GENO BG process for the production of Brontide butylene glycol

distinct production processes will help personal care manufacturers determine how their products affect the environment.

Methods Used for Assessing the Life Cycle of Brontide and Petroleum-Based 1,3-BG

The LCA for these production processes was performed using standard methods and procedures specified by the requirements and guidelines in ISO 14044. The steps of the life cycle relevant to the production processes include raw material extraction, processing, chemical production, end-product production, and the up- and downstream activities involved (e.g., energy, process chemicals, waste management, etc.). A detailed inventory of inputs and outputs of each of these steps was modeled based on representative data available for current technologies. The LCA model was created using the GaBi 8 software system for life cycle engineering and reviewed by three independent experts [Arpad Horvath, PhD (Independent Consultant); Susan Jenkins, PhD (Innovative Genomics Institute, University of California, Berkeley); and Julie Sinistore, PhD (WSP USA Inc.)].

Using this model, the impact of the production processes for Brontide and petroleum-based 1,3-BG were assessed based on seven well-established environmental metrics described as:

- Global Warming Potential (GWP100) [4]
- Primary Energy Demand (PED) and Primary Energy Demand from Non-Renewable Sources (PENRE) [5]
- Eutrophication Potential (EP) [1,2]
- Blue Water Consumption (BWC) [3]
- Ozone Depletion Potential (ODP) [1,2]
- Acidification Potential (AP) [1,2]
- Smog Formation Potential (SFP) [1,2]

Each of these metrics are described in **Tab. 1**.

The Limitations of LCA

The LCA used geographic averages for the analysis of the bio-based production process, which could vary depending on specific crops used as feedstock and the areas where they are cultivated and processed. In addition, transportation distances were assumed for all production processes but will likely vary compared to the process and logistics used at specific facilities.

Similarly, while LCA is intended to provide a very complete view of environmental impact, in many situations the GWP100 is considered the most relevant and impactful

Impact Category	Description
GWP100 (Global Warming Potential) [1]	A measure of greenhouse gas emissions, such as CO_2 and methane.
PED (Primary Energy Demand) and PENRE (Primary Energy Demand from Non-Renewable Sources) [4]	A measure of the total amount of primary energy extracted from the earth.
EP (Eutrophication Potential) [2,3]	Includes the potential impacts of high levels of macronutrients, such as nitrogen and phosphorus.
BWC (Blue Water Consumption) [5]	A measure of the net intake and release of fresh water across the life of the product system.
ODP (Ozone Depletion Potential) [2,3]	A measure of air emissions that contribute to the depletion of the stratospheric ozone layer.
AP (Acidification Potential) [2,3]	A measure of emissions that cause acidifying effects to the environment.
SFP (Smog Formation Potential) [2,3]	A measure of emissions of precursors that contribute to ground level smog formation (mainly ozone O_3), produced by the reaction of volatile organic compounds and carbon monoxide in the presence of nitrogen oxides under the influence of UV light.

Tab. 1 Impact category descriptions

(generally thought of as the greenhouse gas equivalent). All impact factors are presented in this study, as some factors may be important in specific situations or geographies.

The Effect of 1,3-BG Production on Environmental Impact Categories

Using the input/output data collected for each step of the Brontide and petroleum-based 1,3-BG manufacturing process, the relative impact on each environmental category was determined. To compare the effect of each pathway on the various impact categories analyzed, the absolute impact values for the petroleum-based production pathway were normalized to the impact values for the GENO BG process used to make Brontide (**Tab. 2**).

Global Warming Potential and Use of Non-Renewable Resources

Compared to the petroleum-based production of 1,3-BG, the production of Brontide was found to have approximately 50% lower impact on both GWP100 and PENRE metrics (**Fig. 2, Tab. 2**). Emissions that contributed to the GWP from the petroleum pathway were due primarily to production of acetaldehyde starting material and energy usage in the production process, whereas in the GENO BG process, the primary contributors to GWP were feedstock cultivation, fermentation and biogenic process emission of CO_2. Not surprisingly, the petroleum production of 1,3-BG exhibited a far greater impact on PENRE, primarily due to the use of non-renewable natural gas in feedstock and auxiliary materials production (**Tab. 2**).

Reduction in both global warming potential and use of non-renewable resources is an important finding and a significant advantage of the bio-based production process, as both are of great societal importance. Thus, the use of more sustainable production processes in the cosmetics industry can help address global environmental concerns.

The Complications of Corn Feedstock Cultivation

In contrast, the bio-based production process for Brontide showed a greater impact than the petroleum-based 1,3-BG production pathway based on the other environmental metrics analyzed. The greater relative effect of Brontide production on the AP, EP, SFP and BWC metrics was primarily due to emissions from, and indirect activities related to, the cultivation of the plant-based feedstock, specifically corn (**Tab. 2**). The effect of Brontide production on these environmental

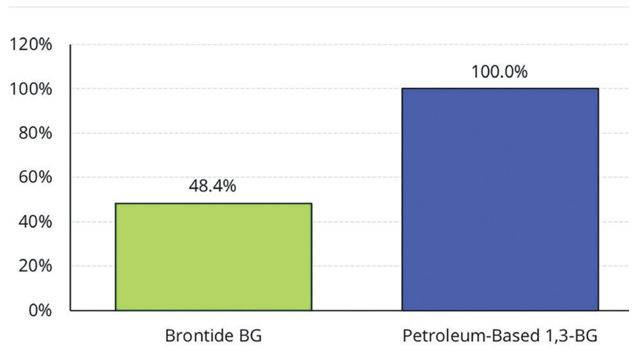

Fig. 2 Relative impact of 1,3-BG production on global warming potential, including biogenic carbon

Impact Category	Units	Absolute Impact		Relative to GENO BG Production Process	
		Brontide BG	Petroleum-Based 1,3-BG	Brontide BG	Petroleum-Based 1,3-BG
GWP100 (Global Warming Potential)	kg CO_{2e}	1.86	3.78	100%	203% (103% higher)
PENRE (Primary Energy Demand from Non-Renewable Sources)	MJ	58.5	109	100%	186% (86% higher)
EP (Eutrophication Potential)	kg N_e	1.35E-02	4.38E-04	100%	3% (97% lower)
BWC (Blue Water Consumption)	kg	332	24.1	100%	7% (93% lower)
ODP (Ozone Depletion Potential)	kg CDC-11_e	4.11E-12	7.01E-13	100%	17% (83% lower)
AP (Acidification Potential)	kg SO_{2e}	1.28E-02	6.40E-03	100%	50% (50% lower)
SFP (Smog Formation Potential)	kg O_{3e}	2.08E-01	1.32E-01	100%	63% (37% lower)

Tab. 2 Impact categories relative to GENO BG production process

metrics will vary by geography, and careful site selection could help to minimize the reported results for these secondary metrics.

Fertilizer used for the cultivation of corn is rich in organic nitrogen (NO_X), sulfur dioxide (SO_2) and phosphate ($PO4^{-3}$), and runoff into freshwater rivers and streams can have a significant environmental impact on soil acidification and eutrophication in farming areas. In reality, however, soil acidification tends to be a concern in only a very narrow set of corn-producing regions in Europe and the U.S., where the pH of soil is already very low. The greater impact of the bio-based pathways on EP, due to the use of fertilizer for corn cultivation; SFP, due to emissions from tractors used for corn cultivation; and BWC, due to corn irrigation and evaporative loss, are considered relevant to this study, although they are an estimate based on available input and output values. In reality, the degree of environmental impact could be minimized based on a variety of factors in the production process.

Ozone Depletion Potential

Lastly, the ODP results of the bio-based process exceeded the petroleum one. However, these results were six orders of magnitude lower than the other impact categories analyzed (**Tab. 2**), and hence deemed inconsequential, when absolute values of each pathway were normalized to TRACI 2.1 US person-equivalents. Therefore, while ozone depletion can have a substantial negative effect on animal and plant life, differences in ODP results between pathways are not considered relevant to the overall conclusions on environmental superiority of one pathway over another.

The Realities of Petroleum-Based and Bio-Based Pathways for 1,3-BG Production

The petroleum-based pathway for 1,3-BG production exceeded the bio-based pathway for Brontide production in both GWP100 and PENRE metrics. Increases in both of these important impact categories are of great environmental and societal importance, as they could have irreversible effects on human life, the environment and conservation. While the bio-based pathway was found to have a greater effect on the other metrics studied, both AP and ODP were considered to be irrelevant. As the benefits of the bio-based production process for 1,3-BG are realized, lower emissions of SFP, EP, and BWC could also be realized through optimization of specific steps in the production process. When compared with each other, the bio-based process for 1,3-BG production was shown to pose less environmental impact than the conventional petroleum-based process. Genomatica hopes this LCA will help personal care and cosmetics formulators choose ingredients that have a reduced environmental impact and help product manufacturers work toward a more sustainable future.

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