CL 304
Chemical Process Technology

LIFE CYCLE ASSESSMENT OF A PETROCHEMICAL AND A BIOBASED MATERIAL

Group: 31

Sugam Barman	**210107084**
Rajat Singhal	**210107100**
Nandini Kathyayan	**210107101**
Prakash Kumar	**210107103**

INTRODUCTION

The escalating global demand for fuels, chemicals, and materials, traditionally met by fossil fuel-based feedstocks, has led to significant environmental concerns, notably greenhouse gas emissions and fossil fuel depletion. This scenario underscores the urgent need for sustainable alternatives that can reduce our reliance on fossil fuels and mitigate their environmental impacts. Lignocellulosic biomass, an abundant and environmentally benign feedstock, has emerged as a promising candidate in this regard. It offers a renewable source for the production of fuels, versatile platform chemicals, and biobased plastics, drawing considerable attention towards technologies that harness its potential.

Among the various products derived from lignocellulosic biomass, 2,5-furandicarboxylic acid (FDCA) stands out as a promising biobased plastic monomer. FDCA serves as a sustainable alternative to petroleum-derived terephthalic acid (TPA) in the polymer industry, finding applications in the production of polyethylene furanoate (PEF), a bioplastic with properties comparable to or better than polyethylene terephthalate (PET).

The production of FDCA from biomass involves a series of catalytic conversions, highlighting the shift towards renewable resources in the polymer industry.

However, the transition from petrochemical to biobased materials is not without challenges. Biorefineries, which process biomass into a spectrum of bioproducts, face economic hurdles such as high capital investment and the complexity of biomass constituents. To enhance the economic feasibility of biorefineries, it is crucial to integrate processes for the production of high-value-added chemicals. This approach not only improves the economic outlook but also contributes to the sustainability of biobased material production.

Environmental sustainability is another critical aspect of biobased material production. While biorefineries offer a greener alternative to traditional petroleum refineries, their environmental impact must be thoroughly assessed to ensure truly sustainable development. Life-cycle assessments (LCAs) play a vital role in this context, evaluating the environmental impacts of biorefinery processes from resource extraction to product consumption. By considering various environmental impact categories, LCAs help identify areas for improvement and guide the development of more sustainable biorefinery processes.

PRODUCTION PROCESS

FDCA Production:

Cellulose to FDCA Conversion via HMF:

The conversion of cellulose to 2,5-furandicarboxylic acid (FDCA) via 5-hydroxymethylfurfural (HMF) involves several critical steps. Initially, cellulose, separated with a 3% loading in solvent, undergoes dehydration to yield HMF, achieving a significant 42% yield.

This process occurs using a tetrahydrofuran (THF)/water solvent (90:10 mass ratio) containing dilute sulfuric acid (20 mM) as a catalyst, operating at 483 K and 68 atm pressure with a residence time of 0.75 h.

The presence of water in the THF solvent significantly impacts HMF yield, with a 10% water content yielding the highest results. THF, as a polar aprotic solvent, enhances HMF yield compared to alternatives like γ-valerolactone (GVL), dimethyl sulfoxide, and 1,4-dioxane in the presence of sulfuric acid. Additionally, the low boiling point of THF (339 K) makes the separation process energy-efficient and economical. Furthermore, humins derived from cellulose degradation are converted to activated carbon during regeneration using oxygen at a high temperature (873 K) with an adsorption bed filled with activated carbon.

Subsequently, FDCA is obtained from HMF in an impressive 93.6% yield through oxidation using a GVL/water solvent (50:50 mass ratio) on a 5% Pt/C catalyst at 383 K and 40 atm pressure.

TPA production:

The process involves three main stages: oxidation, crude terephthalic acid (CTA) recovery, and purification. In the oxidation stage, p-xylene is oxidized to terephthalic acid in the presence of acetic acid solvent and a catalyst solution. The majority of the product is precipitated, while unreacted p-xylene, acetic acid, and water are partially vaporized and sent to a scrubber column for recovery. Residual gas from the scrubber is combusted to dispose of volatile organic compounds. In the crude terephthalic acid recovery stage, the CTA slurry undergoes crystallization, centrifugation, and drying. Solvent streams recovered are purified for water removal before recycling to the oxidation reactor. The dry CTA then undergoes further purification to remove impurities. Finally, in the purification stage, CTA is dissolved in hot water and subjected to hydrogenation to convert undesired impurities into soluble compounds. After solid-liquid separation, the effluent undergoes a second crystallization and centrifugation to separate PTA crystals from mother liquor. Some mother liquor is recycled to the oxidation reaction, converting dissolved hydrogenated compounds back to terephthalic acid, and the remaining PTA wet cake is dried to obtain the final PTA product.

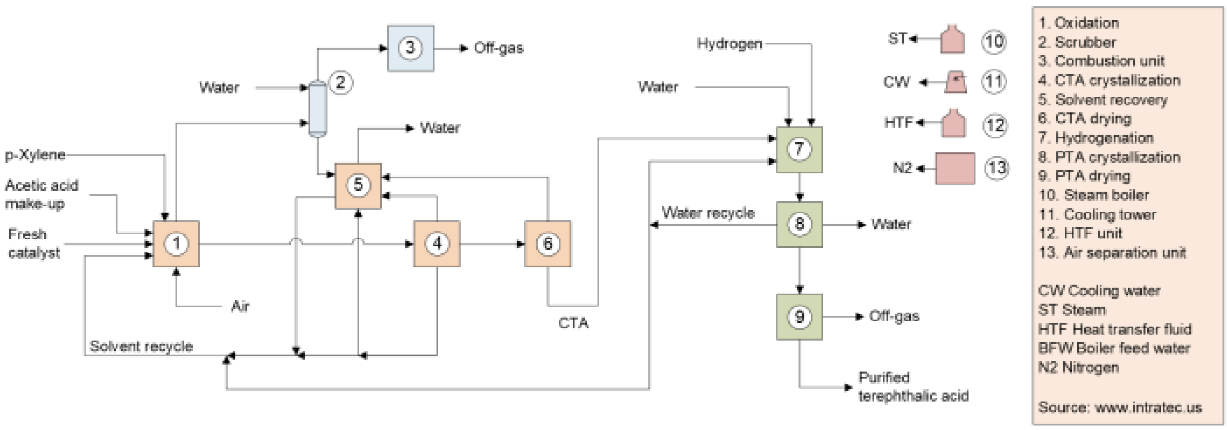


Fig. Process flow diagram of the TPA production

METHODS

Life-Cycle Assessment Methodology:

The Life Cycle Assessment (LCA) framework is a systematic methodology employed to evaluate the environmental impacts of a product or process throughout its entire life cycle. It provides a structured approach for assessing sustainability, indispensable in today's environmentally conscious landscape. Comprising stages such as goals and scope definition, inventory analysis, impact assessment, and interpretation, this framework serves as a vital tool for decision-making, enabling stakeholders to make informed choices towards achieving environmental sustainability goals.

Goal and Scope Definition:

It includes outlining of what's being studied, why it matters, and how it'll be done. It's like mapping out the journey before a road trip, clarifying the destination, route, and purpose to ensure a focused and meaningful assessment.

Inventory Analysis:

The inventory analysis involves compiling all inputs and outputs associated with the production process. This includes raw materials, energy inputs, emissions, byproducts, and waste. The inventory is comprehensive, capturing the flow of materials and energy through the system and quantifying them for subsequent impact assessment.

Impact Assessment:

The impact assessment phase evaluates the potential environmental impacts using established categories such as climate change, fossil depletion, and others. This study focuses on climate change and fossil depletion as key indicators, quantifying the greenhouse gas emissions and the depletion of fossil resources associated with each production process.

Interpretation:

The interpretation phase involves analyzing the results to identify the most significant contributors to environmental impacts. This step is crucial for understanding the potential for reducing environmental burdens and for making informed decisions about process improvements.

Technoeconomic Analysis (TEA) Methodology:

The TEA is a critical component of the study, aiming to determine the economic viability of the production process. It involves calculating the minimum selling price (MSP), which is a key metric for assessing the competitiveness of the product against its counterpart. The MSP is the price at which the product must be sold to achieve a net present value of zero over the lifetime of the project, considering all capital and operational expenses. It is calculated based on the capital and operating costs associated with the production process. This includes the costs of raw materials, utilities, labour, maintenance, and depreciation of equipment. The MSP is influenced by various factors, including the scale of production, process yields, and market prices for feedstocks and byproducts.

Implementation of LCA in production process

Goals and Scope:

The LCA begins with a clear definition of its goal and scope. The goal of LCA in this study is to compare the environmental impacts between biomass- derived FDCA and petroleum-derived TPA productions. The scope includes all stages from raw material extraction to the final product, with a cradle-to-gate approach. The functional unit for comparison can be set as 1 kg of the produced material, ensuring a consistent basis for comparison between the biobased and petrochemical pathways.

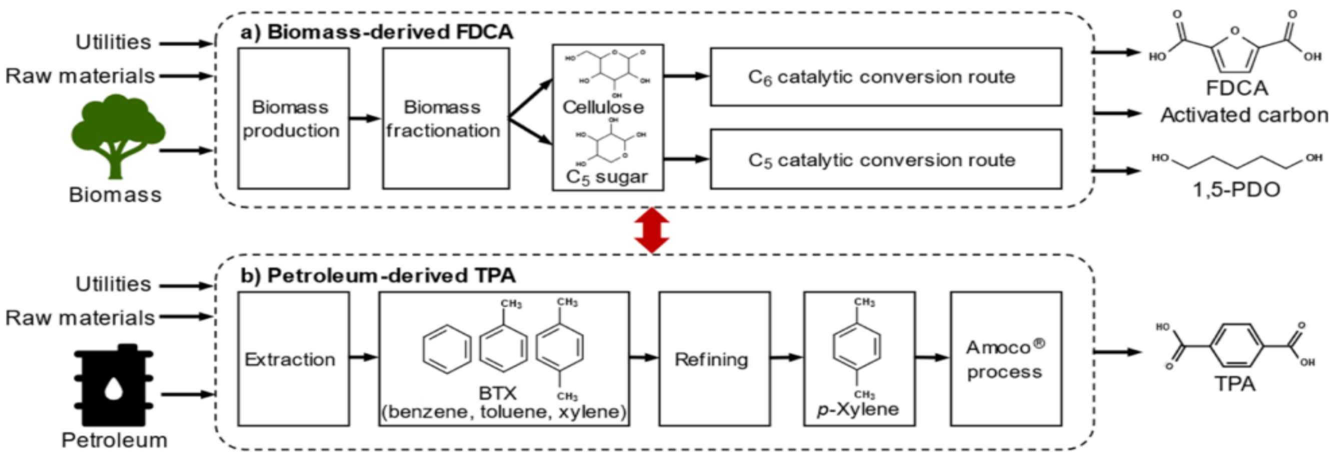


Fig. shows the system boundaries to produce both plastic monomers.

Inventory Analysis:

In the production of petroleum derived TPA, it takes 0.66 kg of xylene to yield 1 kg of TPA, as indicated in the table below. Conversely, in biomass derived FDCA production, 6.74 kg of biomass is required to produce 1 kg of FDCA. Additionally, the process yields 0.65 kg of 1,5-PDO and 0.63 kg of activated carbon as coproduct and byproduct, respectively. Waste products discharged include gypsum and ash in FDCA production, and hydrocarbons, NMVOC, particulates, incineration residue, and hazardous waste in TPA production.

FDCA				TPA			
input		output		input		output	
biomass (kg)	6.74	FDCA (kg)	1	H_2O (m^3)	0.00034	TPA (kg)	1
THF (kg)	0.06	1,5-PDO (kg)	0.65	AA (kg)	0.05	hydrocarbons (kg)	0.00038
H_2SO_4 (kg)	0.21	activated carbon (kg)	0.63	chemical factory (p)	4.0×10^{-10}	NMVOC (kg)	0.00011
heavy oil (kg)	0.03	ash (kg)	0.68	electricity (kW h)	0.47	particulates (kg); <2.5 μm	0.00002
$Ca(OH)_2$ (kg)	0.07	CO_2 (kg)	1.52	heat (MJ); natural gas	0.46	particulates (kg); >10 μm	0.00003
NaCl (kg)	0.05	gypsum (kg)	0.17	heat (MJ); other than natural gas	1.2	particulates (kg); >2.5 μm, < 10 μm	0.00004
H_2 (kg)	0.07	coke (kg)	0.06	N_2 (kg)	0.049	H_2O (m^3)	0.00022
O_2 (kg)	1.43	H_2O (m^3)	0.001	NaOH (kg)	0.0015	incineration residue (kg)	0.006
heat (MJ); natural gas	1.42			steam (kg)	0.64	hazardous waste (kg)	0.0002
electricity (MJ); natural gas	7.02			H_2O (kg)	0.43		
				xylene (kg)	0.66		

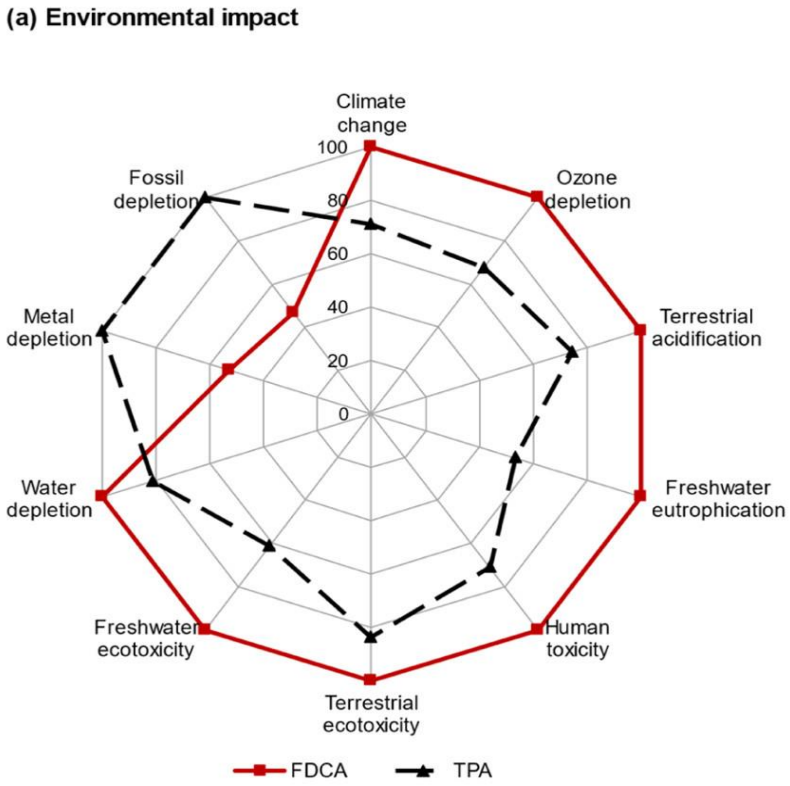
Table: Process Input/Output Values for Biomass-Derived FDCA and Petroleum-Derived TPA

Impact Assessment:

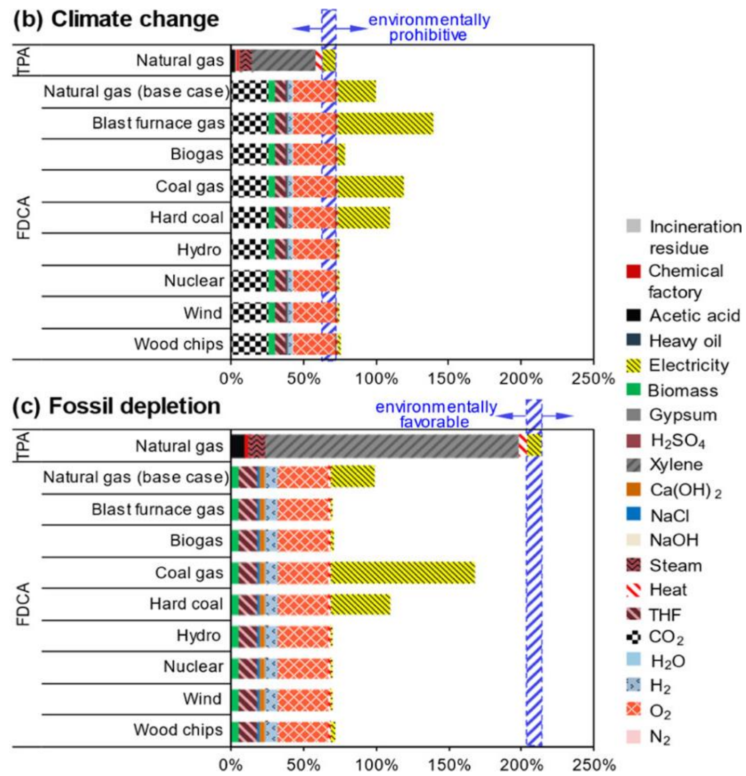
The environmental impacts of producing 1.0 kg of FDCA from biomass and 1.0 kg of TPA from petroleum were assessed across ten standardized categories. These categories include:

- Chemical Change: Evaluates alterations in chemical composition
- Fossil Depletion: Measures the depletion of finite fossil resources
- Metal Depletion: Assessing the depletion of metal resources
- Water Depletion: Evaluating the consumption of water resources
- Freshwater Ecotoxicity: Examining the toxic effects on freshwater ecosystems
- Terrestrial Ecotoxicity: Assessing the toxic effects on terrestrial ecosystems
- Human Toxicity: Measuring the potential toxicity to human health
- Freshwater Eutrophication: Evaluating nutrient overloading in freshwater bodies
- Terrestrial Acidification: Assessing acidifying effects on land ecosystems
- Ozone Depletion: Measuring impacts on the ozone layer.

These categories provide a comprehensive framework for evaluating the environmental footprint of FDCA and TPA production processes, aiding in informed decision-making towards more sustainable practices.



The primary factors influencing Chemical Change (CC) and Fossil Depletion (FD) in the two production processes were determined as shown in the figure below. In the case of biomass derived FDCA production using natural gas for electricity generation, serving as the baseline at 100%, with other values calculated relative to this benchmark.



Interpretation:

The assessment of environmental impacts considered the raw materials utilized in FDCA and TPA production. Altering the production methods of FDCA's raw materials could potentially enhance its environmental performance. However, since the raw materials for FDCA and TPA differ, attention can be directed towards examining the shared aspect of power generation. Electricity generation, relevant to both processes, is analysed for its implications on Chemical Change (CC) and Fossil Depletion (FD), facilitating a comparison of the environmental impacts between the two products.

RESULTS

LCA Results:

Upon going through the entire LCA process, the following results could be concluded:

- In the base case, biomass-derived FDCA was 29% higher in Chemical Change and 53% lower in Fossil Depletion when compared to petroleum-derived TPA.
- Electricity and Xylene play significant roles in the production processes of biomass-derived FDCA and petroleum-derived TPA, respectively. Consequently, the production of TPA from petroleum sources does not significantly mitigate environmental impacts related to carbon emissions and fossil fuel dependence, as it does not effectively reduce the feedstock required to produce a specific quantity of TPA.
- Eight renewable energy resources were considered for electricity generation:

Energy Sources	% Climate Change Impact (Compared to natural gas 100%)	% Fossil Depletion Impact (Compared to natural gas 100%)
Blast Furnace Gas	140	70
Biogas	79	71
Coal Gas	119	168
Hard Coal	109	111
Hydropower	74	70
Nuclear Power	74	70
Wind Power	75	71
Wood Chips	67	73

TEA Results:

The Minimum Selling Price (MSP) analysis reveals key sensitivities for Furan dicarboxylic Acid (FDCA) production. A 20% increase in Total Capital Investment (TCI) resulted in a substantial 30.1% increase in FDCA's MSP. Conversely, a 20% decrease in TCI led to a notable 30.4% decrease in FDCA's MSP. Similarly, a 20% reduction in the discount rate caused a significant 26.6% decrease in FDCA's MSP. Moreover, a 20% reduction in feedstock costs led to a notable 16.4% decrease in FDCA's MSP, primarily due to the utilization of expensive feedstock (US$125/ton, white birch) and a large plant size (2000 ton/day). Conversely, factors such as equity, natural gas price, and tetrahydrofuran (THF) price have a modest impact on FDCA's MSP, causing less than a 7% increase or decrease.

Overall, it was found that MSP for per ton FDCA was 29% lesser than per ton of TPA which indicates that FDCA (biobased) is an economically viable alternative to TPA (petroleum based).

CONCLUSION

In conclusion, our analysis of Techno-Economic Analysis (TEA) and Life Cycle Assessment (LCA) results highlights the economic advantages of biomass-derived Furan-dicarboxylic Acid (FDCA) production over petroleum-derived Terephthalic Acid (TPA) production. However, we observed that FDCA production exhibited less favourable environmental impacts, primarily due to high electricity consumption. Nevertheless, by transitioning to renewable sources for electricity generation, such as biogas, woodchips, or renewable energy technologies like hydro, nuclear, and wind power, the environmental performance of biomass derived FDCA production can be significantly enhanced. Furthermore, exploring alternative feedstocks like corn stover or organic waste could improve both the economics and sustainability of the process. These findings underscore the potential for implementing innovative approaches to mitigate environmental impacts while ensuring the economic viability of biomass-derived plastic monomer production.

REFERENCES

- Miller, S.; Shemer, H.; Semiat, R. Energy and environmental issues in desalination. Desalination 2015, 366, 2– 8, DOI: 10.1016/j.desal.2014.11.034
- Dhyani, V.; Bhaskar, T. A comprehensive review on the pyrolysis of lignocellulosic biomass. Renewable Energy 2018, 129, 695– 716, DOI: 10.1016/j.renene.2017.04.035
- Saini, J. K.; Saini, R.; Tewari, L. Lignocellulosic agriculture waste as biomass feedstocks for second-generation bioethanol production: concepts and recent developments. 3 Biotech 2015, 5, 337– 353, DOI: 10.1007/s13205-014-0246-5
- Won, W.; Maravelias, C. T. Thermal fractionation and catalytic upgrading of lignocellulosic biomass to biofuels: Process synthesis and analysis. Renewable Energy 2017, 114, 357– 366, DOI: 10.1016/j.renene.2017.07.023
- Life-Cycle Assessment of Biorefineries 1st Edition - December 20, 2016, Editors: Edgard Gnansounou, Ashok Pandey