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Environmental assessment of the catalytic arabinose oxidation

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ABSTRACT

Oxidation of arabinose to arabinoic acid is an innovative way to valorize local biomass to a high add value product. Previously done experiments on oxidation of arabinose to arabinoic acid with molecular oxygen were used to determine the optimum reaction conditions, scale-up the process and analyse the techno-economic aspects. These results were utilized to analyse the environmental impact of the scaled-up process during its lifetime using the life cycle assessment (LCA) methodology. SimaPro software combined with the impact assessment method IMPACT 2002+ were applied. The results revealed that heating seems to be the largest contributor to the environmental impact even if the reaction is performed under rather mild conditions (70ºC). This highlights the importance of reducing the energy consumption via efficient heat integration.

Keywords: Catalyst, LCA, Biomass

INTRODUCTION

The global transition toward sustainable chemical processes has underscored the importance of assessing the environmental impacts of emerging industrial technologies. One such process, the catalytic oxidation of arabinose to arabinoic acid, has gained attention for its diverse applications in the pharmaceutical, cosmetic, and food industries due to the functional properties of arabinoic acid as a platform chemical [1, 2].

Gold-based catalysts have been shown to be effective in achieving high sugar conversion and sugar acid selectivity under optimal conditions, especially in a slightly basic environment [3]. However, the environmental impact of scaling up this process needs to be carefully investigated. This is especially true with respect to energy-intensive operations such as heat generation and wastewater treatment.

Life Cycle Assessment (LCA) is a well-established framework for evaluating the environmental performance of chemical processes by systematically analyzing their impact across categories such as human health, ecosystem quality, climate change, and resource use. The IMPACT 2002+ methodology, a widely recognized LCA framework [4], integrates midpoint and endpoint impact categories, enabling a detailed analysis of environmental trade-offs associated with chemical processes. By applying this methodology, the present study aims to evaluate the environmental impact of catalytic oxidation of arabinose to arabinoic acid, focusing on critical hotspots such as heat generation and wastewater treatment.

This research employs a large-scale process model designed in Aspen Plus to simulate the production of arabinoic acid, offering insights into energy consumption, material flows, and waste streams. Specifically, the study investigates the contributions of heat generation and wastewater treatment to the overall environmental footprint of the process, identifying opportunities for optimization and mitigation. The results will pave a way for developing strategies for reducing emissions, minimizing resource depletion, and improving the sustainability of arabinoic acid production, thereby contributing to the broader goal of sustainable industrial chemistry and process technology.

METHODOLOGY

Oxidation of Arabinose

The selective oxidation of arabinose over gold catalysts has been studied extensively to optimize reaction conditions. The process was carried out isothermally at atmospheric pressure in a semi-batch mode, with variations in temperature, pH, and catalytic properties to achieve the best results.

The primary product, arabinoic acid, is obtained via the intermediate arabinolactone. This final product, the sugar acid, and its derivatives are valuable compounds finding applications in the cosmetic, food, and pharmaceutical industries, offering a competitive price and versatility. Figure 1 illustrates the reaction pathway, highlighting the transformation of arabinose to arabinoic acid via arabinolactone.

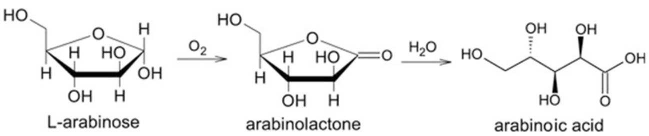

Figure 1. The reaction scheme for selective catalytic oxidation of arabinose (adapted from [5]).

The experimental studies reported in [6, 7] demonstrated that in acidic media, the reaction resulted in only 23% conversion of arabinose after 200 minutes, with 46% selectivity towards the desired product, arabinoic acid. Significant amounts of the intermediate compound, arabinolactone, were formed under these conditions. In contrast, slightly basic conditions (pH 8–9) led to the complete conversion and total selectivity for arabinoic acid within the same time frame. The temperature elevation was observed to enhance reaction activity but also promoted formation of the undesired byproducts.

Utilization of a continuous reactor can be challenging because the pH control is not easy, however, it was shown in [8] showed that continuous sugar oxidation could be carried out in a plug-flow reactor without the need for a pH control alongside the whole reactor. Moreover, it was reported that selectivity in the plug-flow reactor was similar to that in the batch reactor, 94% and 99%, respectively.

Process Design and Modeling

Process design and modeling were conducted in Aspen Plus V11, following the methods used in similar studies previously [9–11]. As the properties of some compounds were not available in the Aspen database, Aspen Properties module was used to estimate the required parameters. The Peng-Robinson equation of state (EoS) was applied to calculate the phase equilibrium [13]. The reactor was modeled using Aspen PFR blocks, in accordance with Ranade et al. [12], who applied plug flow models for trickle bed reactors. Arabinoic acid properties, unavailable in the database, were added via the user-defined compound wizard after their estimation with the Joback method [13], while other parameters were computed with Aspen Properties. The developed flowsheet is

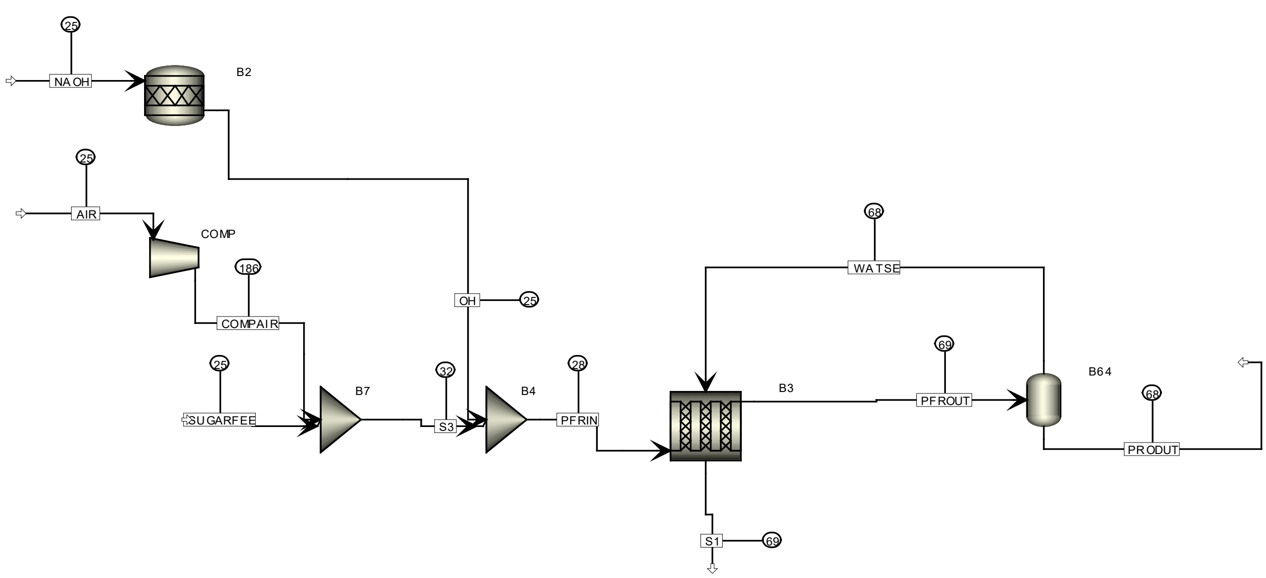

Figure 2. Flowsheet of arabinoic acid production via catalytic oxidation of arabinose

Table 1. Summary of the main operating conditions

pH	Residence time (min)	Temperature (°C)	Pressure (atm)
8	29	60	1

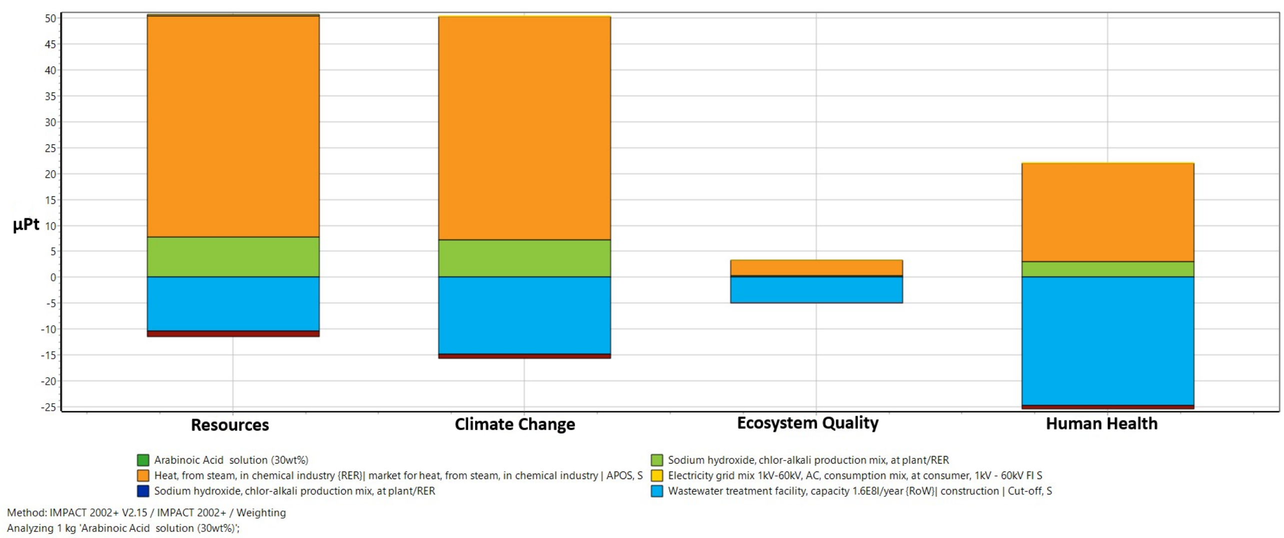

Figure 3. LCA normalized results for the arabinose oxidation.

presented in Figure 2.

Goal and scope

The goal of this study is to investigate the environmental impact of the catalytic oxidation of the arabinose sugar on a supported gold catalyst. This assessment is based on the data generated from the large-scale process model developed using Aspen Plus [10]based on the experimental results generated in laboratory scale [6, 14–16]. In this study, the annual processing capacity of 10 kt of arabinose solution (30 wt%) was considered. The functional unit was taken as 1 kg of arabinoic acid solution (30 wt%). The system boundaries followed a cradle-to-gate approach. SimaPro software was used for this work.

Life Cycle Inventory and Life Cycle Impact Assessment

The life cycle inventory (LCI) data for the system (i.e. chemicals, energy, reactants' consumption) consists of the mass, heat balance, and energy consumption from the simulations using Aspen Plus. The details are reported in our previous publication [10].

Life Cycle Impact Assessment (LCIA) is a phase in the Life Cycle Assessment process where the potential environmental impact associated with a product or process is evaluated. The impact assessment was performed using the impact 2002+ method, originally developed in [4].

RESULTS AND DISCUSSIONS

Figure 3 highlights the environmental impact of arabinose oxidation across four damage assessment categories: Human Health, Ecosystem Quality, Climate Change, and Resource Use, with contributions from specific sources represented as stacked bars.

Heating used in the process emerges as a major contributor to negative impacts in all categories. In the Human Health category, industrial heat processes significantly affect health outcomes, primarily due to emissions and resource-intensive operations. Similarly, for Climate Change, heat generation from industrial sources is the dominant factor driving adverse impacts, reflecting high greenhouse gas emissions associated with these processes. In Resource Use, the production and use of heat in industrial activities lead to substantial resource depletion, further emphasizing its environmental burden. Conversely, the impact of heat-related processes on Ecosystem Quality is relatively minor, though still present.
Wastewater treatment processes generally have a mixed impact. In the Human Health category, they show a slight mitigating effect, likely due to their role in reducing pollutants that would otherwise harm human populations. Similarly, in the Climate Change category, wastewater treatment contributes modestly to mitigating greenhouse gas emissions, though its overall impact is small compared to industrial processes like heat generation.

However, in the Resource Use category, wastewater treatment has a slightly negative impact, most likely due to the energy and materials required for facility operation. The effects on Ecosystem Quality are minimal, indicating that the wastewater treatment has a limited but generally a positive role in addressing ecosystem-related concerns.

The analysis, conducted using the IMPACT 2002+ methodology, underscores the significant role of heat generation in driving environmental and health impacts, particularly in resource use and climate change. This highlights an urgent need for improving the energy efficiency, adopting renewable energy sources for heat generation, and exploring alternative, lower-impact materials in industrial processes to mitigate these effects. Prioritizing these strategies can significantly reduce the environmental footprint of heat-related activities.

CONCLUSIONS

The obtained LCA results show that heat generation is the leading cause of environmental impact across all the major categories, especially resource use and climate change. This emphasizes the urgent need to transition to more energy-efficient systems and integrate renewable energy sources into industrial processes. Heat integration and optimization also play an important role in reducing the energy consumption, thus decreasing greenhouse gas emissions and improving the overall process efficiency.

Wastewater treatment, while essential for mitigating pollution and safeguarding public health, also presents opportunities for further optimization. Enhancing the energy efficiency of treatment systems and integrating renewable energy, such as solar or wind power, into their operation can help offset the environmental burdens associated with these processes.

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