Systems & Control Transactions

**Research Article - Peer Reviewed Conference Proceeding**
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale,
Monika E. Polańska, Filip Logist (Eds.)

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# Life-Cycle Assessment of Chemical Sugar Synthesis Based on Process Design for Biomanufacturing

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## ABSTRACT

The growing demand for sustainable alternatives to petroleum-based products drives the development of biomanufacturing using agriculture-based sugars. However, agricultural sugar production faces significant challenges due to limited production capacity and potential negative environmental impacts. This research examines chemical sugar synthesis as an alternative, assessing its environmental impact with conventional agricultural production methods through life cycle assessment. As formaldehyde serves as a primary substrate in chemical synthesis, four production cases were evaluated—comprising two pathways (conventional methods and $CO_2$ capture and utilization (CCU) technologies), each implemented with either fossil fuels or renewable energy sources. The analysis revealed that semi-batch reactors in chemical synthesis substantially reduce environmental impacts compared to batch reactors. Chemical sugar synthesis demonstrated marked advantages in reducing eutrophication, land use change, and water resources consumption across all formaldehyde production methods evaluated. However, the formaldehyde production process was identified as the determining factor in the overall environmental profile. While chemical synthesis offers environmental advantages in several categories, implementing CCU technologies with renewable energy integration remains necessary to reduce climate change impacts and resource consumption. This work demonstrates the potential of optimized chemical sugar synthesis as an alternative to agricultural sugar production and provides direction for future process development.

**Keywords**: Sugar Synthesis, LCA, $CO_2$ Utilization, Renewable Energy, Batch Process, Catalysis, Environment, Fermentation, Matlab, Modelling and Simulations, Process Design

## INTRODUCTION

### Sugar supply in biomanufacturing

The transition away from dependence on fossil fuels is a critical challenge faced by the global community, and the shift toward the production of materials and energy using biomass as a raw material is accelerating. Currently, the most commonly used sources of reducing power and carbon for the bio-based production of valuable substances are sugars (agriculture-based sugars) obtained from crops such as sugarcane and corn. Bioproduction processes utilizing these sugars have been shown to reduce greenhouse gas emissions compared to fossil fuel-based processes [1]. However, the production volume of agriculture-based sugars is insufficient to meet the massive demand for fuels and chemicals, and excessive industrial use of such sugars risks competing with food supply demands [2]. Additionally, concerns have been raised regarding potential decreases in crop yields due to climate change and supply instability arising from geopolitical risks.

### Sugar synthesis and its life-cycle assessment

Against this background, research has been conducted to synthesize these sugars through catalytic processes that do not rely on agriculture [3]. The chemical synthesis of sugars is achieved by integrating the production of formaldehyde via $CO_2$ reduction with sugar synthesis reactions using formaldehyde as a raw material (Figure 1). Compared to photosynthesis processes that agriculture-based sugars depend on, this method is significantly faster, allows for production near consumption sites, and drastically reduces the consumption of resources such as land and water [4]. As a result, it is expected to address the challenges of raw material supply in bio-production. On the other hand, this method requires more energy compared to conventional agricultural processes, posing challenges in terms of electricity procurement and economic feasibility. Nonetheless, bio-production technologies are essential for the transition to a circular economy, and systems capable of supplying raw materials in large quantities and with stability are equally necessary. Therefore, it is crucial to provide quantitative and objective insights into the changes brought about by the introduction of such technologies, including energy requirements and environmental impacts.

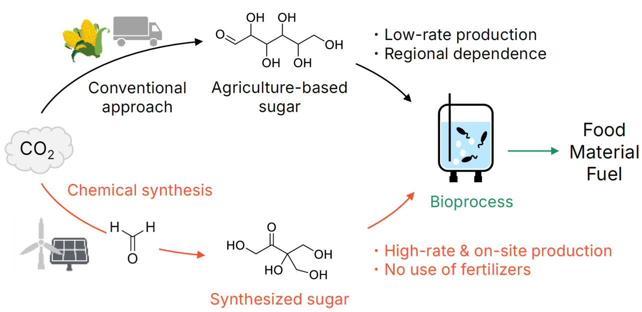


**Figure 1.** A scheme of biomanufacturing using chemically synthesized sugars as the substrates.

In this study, to determine whether the challenges of raw material supply in biomanufacturing can be addressed through the chemical synthesis of sugars, the energy requirements and environmental impacts of each process were evaluated using life-cycle assessment (LCA).

## MATERIALS & METHOD

### Numerical simulation

The time-dependent concentration changes of reactants and products in the chemical reaction were modeled using a set of coupled ordinary differential equations (ODEs). These equations were derived from the reaction rate laws, assuming homogeneous reaction conditions. The system of ODEs was solved numerically using MATLAB (version R2024b, MathWorks, Natick, MA, USA). The ode45 solver, based on an adaptive Runge-Kutta (4,5) method, was employed. The reaction rate constants were taken from the literature [5].

### Life-cycle assessment

#### Goal and Scope Definition

The primary goal of this study is to evaluate the environmental impacts associated with the chemical synthesis of sugar using a simulation-based yield of the reaction. The assessment was conducted following the ISO 14040 and ISO 14044 standards. The functional unit was defined as 1 kg of synthesized sugar, and the system boundary encompassed a "cradle-to-gate" approach, including raw material extraction and chemical synthesis.

#### System Boundaries

The LCA model encompassed four primary stages: raw material acquisition, chemical reaction (modeled using MATLAB to calculate sugar yield), catalyst removal, and product concentration. For the procurement of formaldehyde as a feedstock for chemical synthesis, two methods of production were considered: conventional production from fossil fuels based on the IDEA database, and production via $CO_2$ capture and utilization (CCU) technologies [6]. As the synthesized sugar product is intended to be used directly as a substrate for bioprocesses following concentration of the product [7], no further purification of the sugar product was considered. Infrastructure development, maintenance, and the transportation of raw materials and final products were excluded from the system boundary, as their contributions were deemed negligible for this study.

#### Environmental impact assessment

The life-cycle inventory was calculated using data obtained from the following sources: Material and energy balances were calculated based on stoichiometric equations and simulation results from the material balance and energy consumption for the reaction. Background data such as energy production and chemical manufacturing were sourced from the IDEA ver. 3.4.1 database.

Environmental impacts were assessed using life-cycle impact assessment (LCIA) methods. Global warming potential was evaluated using climate change factors from IPCC 2021 GWP 100a with LULUCF (Land Use, Land-Use Change and Forestry). The other environmental impacts, including eutrophication, land use (transformation), resource consumption, and water resources consumption were assessed using the LIME2 (Life-cycle Impact assessment Method based on Endpoint modeling 2) methodology.

## RESULTS & DISCUSSION

### Kinetic simulation of the formose reaction

The kinetic simulation of the formose reaction were performed using the mathematical model proposed by Socha et al. (1981) [5], which consists of a system of differential equations describing the concentration changes of formaldehyde and carbohydrates (C2-C7) over time. The model incorporates five key reactions: (1) aldol condensation of formaldehyde with sugars, (2) aldol condensation between sugars, (3) retro-aldol reaction of sugars, (4) Cannizzaro reaction, and (5) saccharinic acid formation.

The simulation was performed using MATLAB to solve the coupled differential equations numerically. The results demonstrated that the total yield of sugars (C2-C7) reached 65.2% under the given reaction conditions (40°C, 200 minutes, initial formaldehyde concentration of 4.5% (w/w)) (Figure 2). This value represents the combined yields of various carbohydrates formed through the complex reaction network. The obtained sugar yield was subsequently used as a basis for mass balance calculations in the sugar synthesis process design.

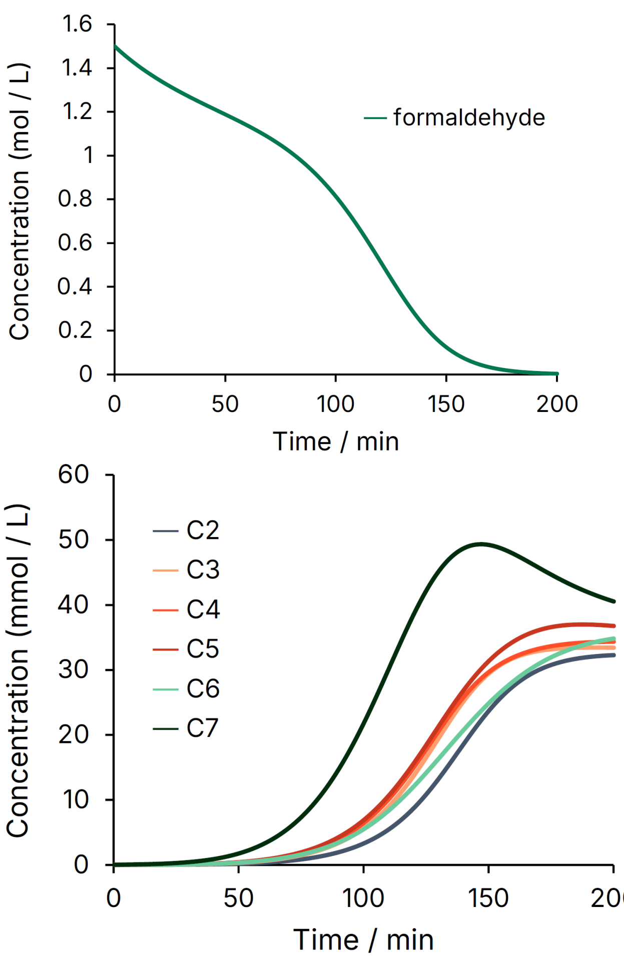


**Figure 2.** Simulation results showing the concentration changes of formaldehyde and each sugar species (C2-C7) during the formose reaction.

## Environmental impact assessment of sugar synthesis

Mass and energy balances were calculated for each process step in the chemical synthesis of sugars, including the thermal reaction, catalyst removal, and the evaporative heating for removal of residual substrate and water solvent. The theoretical energy requirements for heating and evaporation processes were determined using thermodynamic properties. To account for real process conditions, an energy efficiency factor of 70% was applied to calculate the actual energy requirements for each unit operation.

Figure 3 shows the environmental impacts of the sugar synthesis process when using a batch reactor for the formose reaction. The results were categorized into five impact categories: climate change, eutrophication, land use (transformation), resource consumption, and water resources consumption. The impacts were presented as relative contributions (%) of each input: formaldehyde (37% aqueous solution), water, calcium hydroxide, sulfuric acid, and heat energy. As shown in Figure 3, the impact of heat energy was significant in the categories of climate change, land use (transformation), and water resources consumption. The contribution of heat energy was particularly large in these categories, accounting for more than 50% of each impact. In the category of eutrophication, the impact of formaldehyde was dominant, accounting for more than 50% of the total impact. For resource consumption, both formaldehyde and heat energy showed significant contributions.

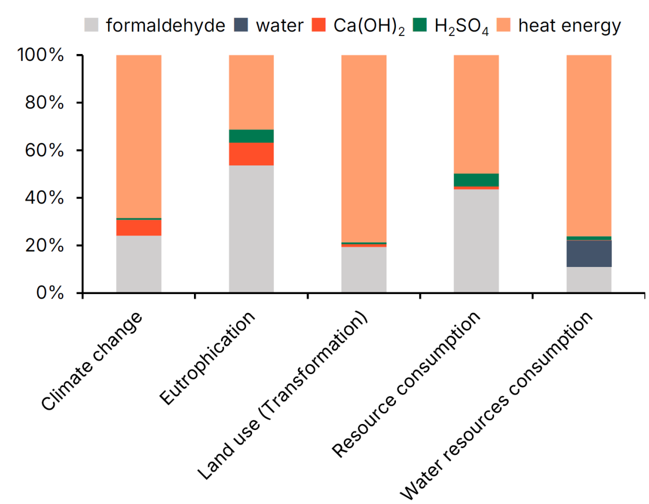


**Figure 3.** Contribution of each input to the environmental impacts (climate change, eutrophication, land use (transformation), resource consumption, and water resources consumption) in the sugar synthesis process using a batch reactor.

Importantly, the formose reaction possesses an autocatalytic reaction cycle [8], allowing for continuous sugar synthesis by continuously adding formaldehyde during the reaction, that is, by adopting a semi-batch reactor. Therefore, the impact on climate change by adopting a semi-batch reactor was evaluated (Figure 4). The vertical axis shows the GHG emissions per 1 kg sugar produced, and the horizontal axis shows the product concentration. It was revealed that by increasing the product concentration through continuous addition of the substrate, the amount of calcium hydroxide used as a catalyst and the energy required for the concentration process can be significantly reduced. For example, increasing the product concentration to 20% (w/w) can reduce GHG emissions by more than 60% compared to the use of a batch reactor where the product concentration was 4.5%. This reduction is mainly attributed to the decreased energy needed for evaporating water in the concentration process due to the higher sugar concentration, as well as the reduced amount of calcium hydroxide used per unit of sugar produced. These findings demonstrate the effectiveness of the semi-batch reactor in improving energy efficiency and reducing the environmental impact of sugar synthesis.

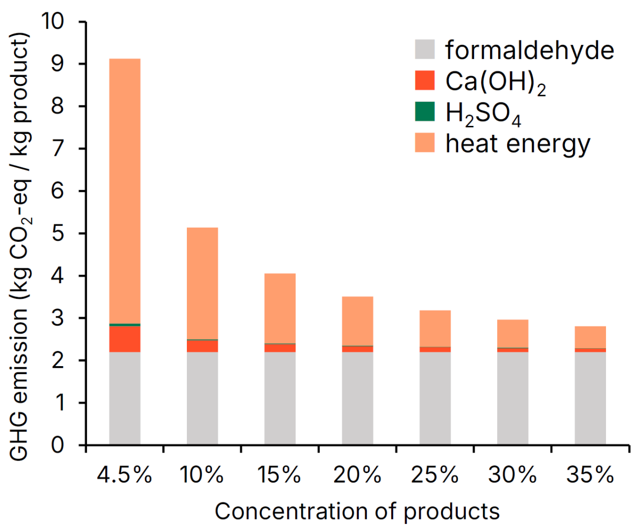


**Figure 4.** Changes in GHG emissions (kg $CO_2$-eq) per input with increasing product concentration when using a semi-batch reactor.

Figure 5 shows the contribution of each impact category when a semi-batch reactor is adopted, and the product concentration is increased to 20% (w/w). As the contribution of heat energy decreased, the contribution of formaldehyde became dominant in each environmental impact. This highlights the significant influence of the formaldehyde production process on the overall environmental performance of sugar synthesis. These findings suggest that improving the manufacturing process of the substrate, formaldehyde, is a crucial factor in reducing the environmental impact of chemical sugar synthesis.

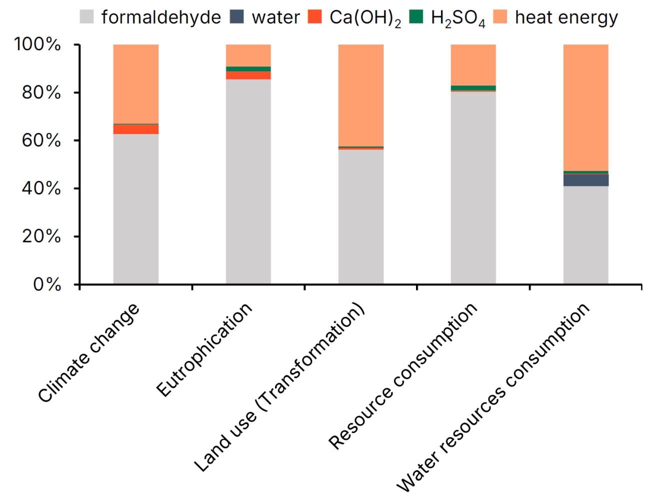


**Figure 5.** Contribution of each input to the environmental impacts (climate change, eutrophication, land use (transformation), resource consumption, and water resources consumption) in the sugar synthesis process using a semi-batch reactor with a product concentration of 20%.

## Changes in environmental impact due to the adoption of $CO_2$ conversion technology

Building upon the previous findings highlighting the significant contribution of formaldehyde to the environmental impact, the environmental impact of formaldehyde production using $CO_2$ as a raw material was evaluated. The assessment employed inventory data from existing literature for the CAMERE process to model $CO_2$ utilization [6]. Figure 6 illustrates a comparison of GHG emissions across different cases. Cases A and B represent conventional formaldehyde production methods. Case A utilized the IDEA database's local heat supply (global) as the emission factor for heat energy, while Case B assumed that heat energy was supplied by renewable energy (geothermal energy). In contrast, Cases C and D represent formaldehyde production via CCU technologies. Case C assumed that the required hydrogen is derived from natural gas, with the heat energy source being the same as in Case A. Case D assumed that the required hydrogen was obtained from water electrolysis powered by geothermal power generation, and also the heat energy was supplied by geothermal. Furthermore, since the carbon source for the sugar produced in Cases C and D was $CO_2$, the calculated emissions took into account the amount of $CO_2$ absorbed.

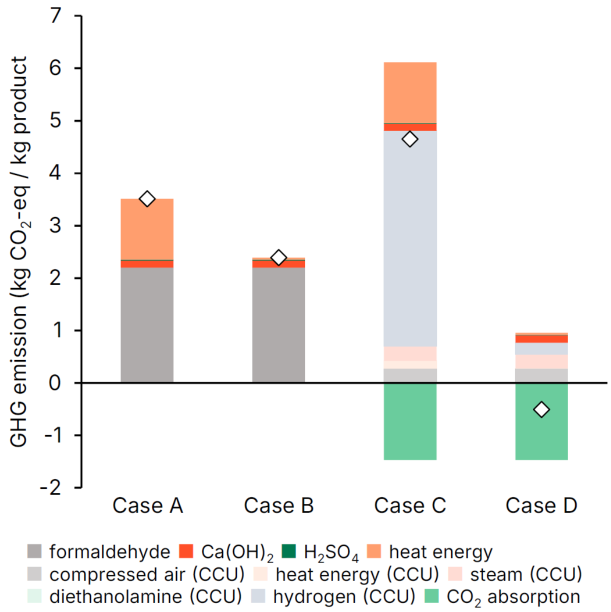


**Figure 6.** Comparison of GHG emissions (kg $CO_2$-eq) per kg of sugar produced under four different cases (Cases A-D). Cases A and B represent conventional formaldehyde production methods, while Cases C and D represent formaldehyde production methods utilizing $CO_2$. Cases A and C assume heat supply mainly from fossil fuels, and Cases B and D assume heat supply from geothermal power generation.

Figure 6 compares the GHG emissions for the four different cases, highlighting the significant impact of the formaldehyde production method. In Case A, which used the current energy supply as energy resources, the GHG emissions were estimated to be approximately 3.5 kg $CO_2$ per 1 kg of sugar. Using renewable geothermal energy for the heat energy in Case B reduced the emissions to around 2.4 kg $CO_2$. However, when $CO_2$ was used as the raw material in Case C, the emissions increased to approximately 4.6 kg $CO_2$, primarily due to the natural gas-derived hydrogen. Despite $CO_2$ uptake, the overall emissions remained high. In stark contrast, Case D, which utilizes hydrogen produced from water electrolysis powered by geothermal energy and uses geothermal energy for heat, achieved a remarkable reduction in emissions, resulting in approximately -0.6 kg $CO_2$. This negative value signifies that the process absorbs more $CO_2$ than it emits (although it is important to note that the synthesized sugar will eventually be emitted as $CO_2$ during its use and disposal, so this does not mean that the emissions are negative over the entire life-cycle). These results clearly demonstrate that while adopting CCU technologies is a promising approach, the introduction of renewable energy is indispensable for maximizing its environmental benefits. Without the integration of renewable energy, the benefits of CCU technologies may be significantly diminished, and could even lead to a higher GHG footprint than conventional methods, as observed in Case C.

## Comparison with agriculture-based sugar

Figure 7 compares the environmental impacts of the four cases (A-D) described in the previous section with those of agriculture-based sugar production across five environmental impact categories. The values are normalized, setting the largest environmental impact among the compared cases to 1 for each impact category. It should be noted that their functional unit differs from that of agriculture-based sugars (glucose in this case) while chemically synthesized sugars are reported to be metabolizable by microorganisms [9] and usable as a raw material for biomanufacturing [7]. The results showed that regardless of the case, the adoption of chemical sugar synthesis technology could significantly reduce environmental impacts in terms of eutrophication, land use (transformation), and water resources consumption. For instance, the impact on eutrophication from chemical synthesis was, at most, approximately 1/10,000th (Case A), and could be as low as approximately 1/24,000th (Case D) of agriculture-based sugar. Similarly, the impact on land use was between approximately 1/70th (Case C) and 1/140th (Case D), and the impact on water resources consumption was between approximately 1/9th (Case A) and 1/30th (Case D) that of agriculture-based sugar. On the other hand, in terms of climate change and resource consumption, the introduction of CCU technologies, premised on the implementation of renewable energy, was essential for reducing environmental impact.

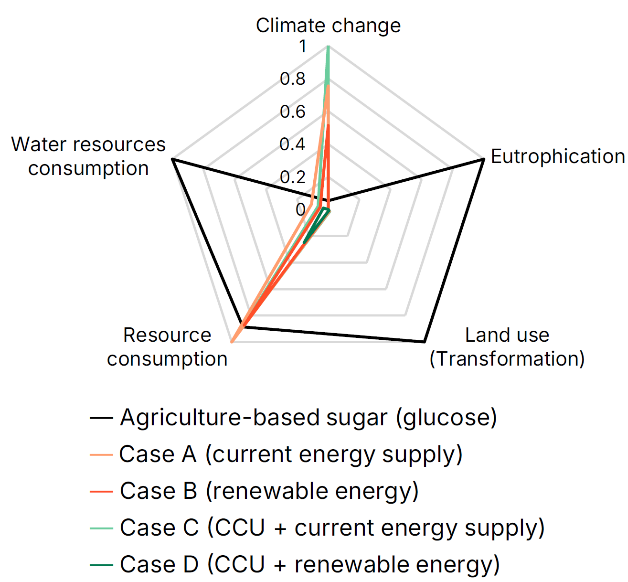


**Figure 7.** A radar chart of indices for all cases of sugar synthesis and agriculture-based sugar, the values of which are normalized as the maximum one in an indicator is set to 1.

## CONCLUSION

This study assessed the environmental impact of chemical sugar synthesis as an alternative to agriculture-based sugar production. The results demonstrated that the chemical synthesis of sugar, particularly when adopting a semi-batch reactor, can significantly reduce environmental impacts in terms of eutrophication, land use, and water resources consumption compared to conventional agriculture-based sugar production. However, the study also highlighted the crucial role of formaldehyde production in the overall environmental footprint. The introduction of CCU technologies for formaldehyde production, premised on the implementation of renewable energy, proved essential for reducing the environmental impact, particularly regarding climate change and resource consumption. Case D, utilizing both CCU and geothermal energy, showed the most promising results among the cases. The findings provide valuable insights for process optimization and future research directions, particularly in the development of more efficient and sustainable formaldehyde production technologies. Further studies should investigate the economic feasibility and scalability of the proposed process, and also focus on a more detailed analysis considering other potential environmental impacts.

The environmental impact of the excessive expansion of agriculture-based sugar utilization has been pointed out in the past. However, as of yet, no replacement methods have been established. In contrast, chemical sugar synthesis is much faster than the agricultural process, and it consumes far fewer resources, such as land and water. This study quantitatively demonstrates the social significance of supplementing sugar production with chemical synthesis processes. Consequently, it is expected to provide new methodologies and perspectives for the field of biomanufacturing, which has been based on the use of agriculture-based sugars, and ultimately for the entire carbon resource recycling system, including food production.

## ACKNOWLEDGEMENTS

This work was supported by New Energy and Industrial Technology Development Organization (NEDO, Grant number JPNP20011), JSPS KAKENHI (Grant Number JP24K23916). Activities of the Presidential Endowed Chair for “Platinum Society” at the University of Tokyo are supported by Mitsui Fudosan Corporation, Sekisui House, Ltd., East Japan Railway Company, and Toyota Tsusho Corporation.

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