Title: Sustainable Production of Acrylic Acid via 3-Hydroxypropionic Acid from Lignocellulosic Biomass

Authors: Sarang S. Bhagwat[1,2], Yalin Li[1,3], Yoel R. Cortés-Peña[1,2], Emma C. Brace[1,3], Teresa A. Martin[1,4], Huimin Zhao[1,4], **Jeremy S. Guest**[1,2,3]

Institutions: [1]DOE Center for Advanced Bioenergy and Bioproducts Innovation (CABBI), University of Illinois at Urbana-Champaign, 1206 W. Gregory Drive, Urbana, IL 61801, USA; [2]Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, 3221 Newmark Civil Engineering Laboratory, 205 N. Mathews Avenue, Urbana, IL 61801, USA; [3]Institute for Sustainability, Energy, and Environment (iSEE), University of Illinois at Urbana-Champaign, 1101 W. Peabody Drive, Urbana, IL 61801, USA; [4]Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, 215 Roger Adams Laboratory, 600 S. Mathews Avenue, Urbana, IL 61801, USA

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Project Goals: The goals of this project were (i) to characterize, under uncertainty, the financial viability (via techno-economic analysis, TEA) and environmental impacts (via life cycle assessment, LCA) of biorefineries producing acrylic acid via 3-hydroxypropionic acid (3-HP) from lignocellulosic feedstocks for the current state of technology as well as across potential technological improvements, (ii) to benchmark the performance of these biorefineries against conventional and alternative production processes, and (iii) to set specific technology performance targets to identify and prioritize research needs.

Abstract Text: Lignocellulosic biomass is a promising renewable feedstock for the sustainable manufacturing of biofuels and bioproducts. Among emerging bioproducts, 3-HP is of particular interest as a platform chemical to produce commercially significant chemicals such as acrylic acid. In this study, BioSTEAM[1]—an open-source platform—was leveraged to design, simulate, and evaluate (via TEA and LCA) biorefineries producing acrylic acid via fermentation of sugars (glucose and xylose) to 3-HP. At the current state of technology, the biorefinery could produce high-purity (>99.5 wt%) acrylic acid at a minimum product selling price (MPSP) of $\$1.83\cdot kg^{-1}$ (baseline) with a range of $\$1.72-2.08\cdot kg^{-1}$ [5^{th}–95^{th} percentiles, hereafter shown in brackets], a 100-year global warming potential (GWP_{100}) of 3.90 [3.42−4.63] kg CO_2-eq$\cdot kg^{-1}$, and a fossil energy consumption (FEC) of 51.4 [43.1−62.1] $MJ\cdot kg^{-1}$. The environmental impacts (GWP_{100} and FEC) for the current state of technology were shown to be significantly lower than those of conventional (fossil-derived) acrylic acid and similar to those of algal glycerol-derived acrylic acid. Advancements in key technological parameters (fermentation yield, titer, and saccharification solids loading) could greatly enhance the biorefinery's performance (MPSP of $\$1.29-1.52\cdot kg^{-1}$ with ~88% probability of market-competitiveness, GWP_{100} of 3.00 [2.53−3.38] kg CO_2-eq$\cdot kg^{-1}$, FEC of 39.9 [31.6−45.1] $MJ\cdot kg^{-1}$). Alternative fermentation regimes (neutral/low-pH fermentation across titer, yield, and productivity combinations) and alternative feedstocks

(first/second generation feedstocks across price and sugar/carbohydrate content) were evaluated to map the sustainability of the biorefinery across the selected design and technology space under uncertainty. Overall, this research highlights the ability of agile TEA-LCA to screen promising biorefinery designs, navigate sustainability tradeoffs, prioritize research needs, and establish a roadmap for the continued development of bioproducts and biofuels.

References

(1) Cortés-Peña, Y.; Kumar, D.; Singh, V.; Guest, J. S. BioSTEAM: A Fast and Flexible Platform for the Design, Simulation, and Techno-Economic Analysis of Biorefineries under Uncertainty. *ACS Sustainable Chem. Eng.* **2020**, *8* (8), 3302–3310. https://doi.org/10.1021/acssuschemeng.9b07040.

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