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Editorial

Effective Assessment Practices for Using Sustainability Metrics: Biomass Processing

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Energy and chemicals are still mostly produced from building blocks obtained from petroleum, coal, and natural gas industries. However, there is incessant demand for these commodities to be produced from sustainable production schemes, and usually, these start with building blocks derived from renewable biobased resources. Biomass is one of these streams that could supply building blocks. Biomass encompasses all feedstock produced by biological organisms and can include, but is not limited to, crop residues, herbaceous energy crops, woody crops, algae and other marine streams, or construction waste. Although present in the pulp and paper industry, biomass processing involves a complex network of operations and processes that are not present in petrochemical production operations. Thus, a clear delineation of the production operations becomes imperative so that all steps involved in biomass transformation are evaluated in terms of their environmental sustainability metrics. These metrics provide an unbiased path to evaluate biomass processing systems. In addition to social and economic considerations, a process is environmentally sustainable relative to an alternative if for similar product yields less chemical and energy inputs are required, while minimizing noxious by-products. Environmental sustainability analysis is critical to identify hotspots, which will in turn highlight additional research needs. This editorial suggests guidelines for quantitative sustainability assessments in manuscripts focused on biomass processing to produce energy and chemicals. The guidelines are based on the types of manuscripts we receive in this area and are focused on the chemical- and biological-engineered processes carried out in biomass processing. Please note that the present guidelines do not cover catalysis as it pertains to biomass processing. Instead, we refer you to a separate *ACS Sustainable Chemistry & Engineering* editorial on sustainability metrics for catalysis and catalytic processes.[1]

GENERAL CONCEPTS

Biomass is processed in a biorefinery, which is a dedicated facility for its conversion to energy, chemicals, and other beneficial products; smooth functioning of a biomass supply chain is needed for its sustainable operation. Before arriving at the biorefinery, biomass must be produced, harvested, collected, processed, and transported. These steps are collectively referred to as the feedstock supply chain and logistics and are like biomass preparation steps carried out in agriculture and pulp and paper sectors. The operations in the feedstock supply chain and logistics could vary widely depending on the biomass type. For example, forest biomass requires planting and thinning as common operations in feedstock production, while fertilizer application and irrigation are common for crop residues production. Regardless of their production operations, biomass must be processed from a "standing in the field or forest" state to a material that is suitable for transportation to the biorefinery through a series of operations, for example, felling, delimbing, bucking, chipping, chopping, and baling. At the biorefinery, processing starts with biomass preparation, typically involving some or all of the following operations: size reduction, drying, sieving, blending, and densification. The specific preparation steps depend on the nature of the biomass as well as the extent of processing required for presentation at the throat of the reactors. Biomass conversion in the biorefinery is achieved through biochemical and thermochemical pathways. A pathway includes specific processes that transform biomass into intermediates and may consist of more general downstream processes required to separate, purify, condition, and upgrade intermediates to their final targeted products. The biochemical pathway includes relatively mature unit operations that encompass chemical or enzymatic deconstruction of starch-based, lignocellulosic, or marine feedstocks into sugars, which can then be fermented into fuels or chemicals at mild temperatures.[2] An example of this pathway includes biomass enzymatic breakdown into monomeric sugars followed by fermentation to ethanol, butanol, and other chemicals. In contrast, the thermochemical pathway employs intermediate to high temperatures, with or without catalysts and other chemicals, to deconstruct biomass into intermediate species, which could be transformed into fuels and chemicals.[3] Examples of this pathway include biomass processing by fast pyrolysis, gasification, and hydrothermal liquefaction to produce intermediate products that are further upgraded to fuel and chemicals. Additional routes, made possible by novel thermo-, electro-, and biocatalytic developments, are emerging. Sustainability assessments of the biomass processing system are more effective when they evaluate all the subsystems holistically.

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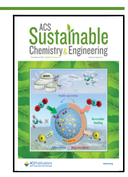

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SUSTAINABILITY METRICS USED IN BIOMASS PROCESSING

Sustainability metrics are useful to compare the intrinsic performance of biomass processes against incumbent alternatives. Thus, in addition to the conversion, yield, and selectivity, we encourage authors to use metrics such as the E-factor and global warming potential (GWP) to quantify the sustainability of their biomass processes. The diversity of the types of processes and operations necessary to transform biomass makes it challenging to prescriptively select a finite set of metrics in this area.[4,5] We encourage the authors to review *ACS Sustainable Chemistry & Engineering* articles as well as other sources to identify suitable metrics for their specific research areas.[4,6] For example, in the biomass supply and logistics area, chemical and energy inputs vary widely based on the feedstock types, production, and logistic operations. Typical energy inputs include the energy required to operate equipment and machineries for growing, harvesting, and in-field processing as well as for transportation. Common chemical inputs include fertilizers, herbicides, and water. While we do not focus on manuscripts that address the sustainability analysis of biomass supply chain and logistics, their energy and chemical use associated with production must be accounted. Chemical and energy inputs in biorefinery operations are generally an important share of overall inputs in biomass processing. Biomass preparation and storage generally require modest chemical inputs. However, size reduction and drying are especially energy voracious steps for biomass preparation and transportation and should be quantified. In the drying step, heat integration is a common strategy implemented to minimize the energy demand by recovering and recycling heat from other parts of the biorefinery. Because biomass is perishable and flammable, moisture, temperature, and fire risks must be monitored and managed during storage; energy inputs should be quantified.

The energy and chemical inputs during the conversion step of biomass processing are significant. In the biochemical platform, biomass pretreatment is needed to improve enzymatic activity. Except for organosolv pretreatments, this step is usually water based. However, after all pretreatment steps, some form of washing is needed, as this improves enzymatic activity. Water usage during pretreatment, washing, and enzymatic hydrolysis should be quantified with appropriate mass-based and other relevant metrics, for example, E-factor.[6] Authors are encouraged to use and report on solvent selection tools to guide their selection. The CHEM21 toolkit is an example of an appropriate solvent selection tool.[7] Disposal of byproducts that are formed during unit operations should be quantified and accounted for. Ideally, biomass disposal would be replaced through byproduct valorization; however, energy, water, and solvent usage should be tallied. The valorization of these byproducts will depend on the energy and costs required for, but not limited to, catalyst synthesis, upgrading process, and product separation and purification steps.

Water will be omnipresent during biochemical fermentation steps, and its use should be quantified through tools such as E-factor. Fermentation processes are very sensitive to temperature ranges, requiring voracious volumes of cooling water, which should be quantified. Fermentation processes usually result in targeted products in diluted form, requiring further downstream processing steps (e.g., fractionation, separation, and recovery). Approaches using CHEM21toolkit[7] are encouraged as they can nudge toward selecting fewer toxic solvents and nonsolvent operations (e.g., membrane filtration and chromatographic separations). Fermentation usually implies carbon dioxide production, which needs to be quantified and, if possible, not released to the atmosphere, implying the design of capture or valorization steps.

In the thermochemical platform, the requirements for energy and chemicals vary greatly. For example, in gas−solid thermochemical processes like fast pyrolysis and gasification, energy inputs are important, with a significant portion heating the conversion reactors to their high temperatures. In these processes, it is common to see process configurations that attempt to generate and recycle heat to offset the energy demand by promoting carbon oxidation reactions. For example, in fast pyrolysis conceptual biorefineries, biochar, the main byproduct, as well as coke formed on a catalyst's surface are combusted to generate heat. It should be noted, however, that this approach affects the overall carbon efficiency into the products since parts of the carbon is diverted to heat generation. In such cases, strategies that valorize the flue gas generated during biochar combustion should be integrated to minimize biogenic carbon waste. Chemical inputs in the gas−solid thermochemical processes are diverse. For example, hydrogen is used to deoxygenate bio-oil, the primary product of fast pyrolysis, either in the conversion reactor or downstream processes. The use of solvents, water, and other chemicals is modest in gas−solid thermochemical processes and is largely concentrated in downstream processes. In contrast, liquid−solid thermochemical processes are typically less energy intensive because they require lower conversion temperatures and less chemical intensive because they are carried out in water or solvents. For example, in hydrothermal liquefaction, important quantities of water and solvents are used during biomass liquefaction into crude oil and separation of crude oil fractions.

Energy and chemical inputs and outputs should be quantified as their quantities are required to compute various sustainable metrics. Additionally, the conversion of biogenic carbon to desired products should be quantified since the biomass carbon can be distributed in numerous products, some of which can exert deleterious environmental impacts. For example, gaseous molecules, such as CO and CO_2, are produced in most thermochemical processes and should be quantified, tracked, and, if possible, recycled to maximize biogenic carbon efficiency and minimize their deleterious environmental impacts. To the extent possible, the elemental balance of C, O, and H should be carried out and optimized toward higher carbon conversion to products. Additionally, heterogeneous catalysis can play a vital role in upgrading biomass-derived molecules to fuels and chemicals but can be deactivated.[8] The sustainability of the heterogeneous catalysts should be reported following guidelines reported in the *ACS Sustainable Chemistry & Engineering* editorial on sustainability metrics for catalysis and catalytic processes.[1]

OVERALL PROCESS ANALYSIS

Techno-economic (TEA) and life cycle (LCA) analyses are two important tools for evaluating the sustainability of both biomass processes and products; however, generic TEA or LCA that do not rigorously evaluate specific process and regional realities are not encouraged. In our context, TEA evaluates the costs, benefits, risks, and uncertainties associated with transforming specific biomass from its "standing in the

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field" state to targeted products and coproducts through explicit processes. Similarly, LCA seeks to quantify environmental impacts over a defined domain, for example, cradle-to-gate, cradle-to-grave, gate-to-gate, and cradle-to-cradle. Both TEA and LCA rely on process or system analyses which provide material and energy inventories necessary to quantify sustainability metrics. TEA and LCA measure sustainability using economic and environmental impact indicators, including, but not limited to, levelized cost of products, cost of waste disposal, greenhouse gas emissions, ozone depletion, acidification, eutrophication, smog formation, energy usage, and ecotoxicity. TEA and LCA assumptions should be carefully evaluated. For example, but not limited to, energy that is needed for a given system can vary in terms of its environmental footprint depending on the regions and sources; similar caveats can also affect water usage. TEA and LCA studies that include uncertainty analysis are also especially encouraged.[9] The use of TEA and LCA is encouraged when evaluating multiple processes integrated into a system.

■ CONCLUSION

Broadly, metrics associated with novel or traditional feedstocks being transformed into energy and chemicals are needed such that the sustainability of these biomass-based processes can be compared to their conventional counterparts. Future production schemes need to be economically viable as well as sustainable. For this, identification of processing hotspots is needed such that they can be addressed and amended through research. We look forward to your feedback and your manuscript submissions to *ACS Sustainable Chemistry & Engineering* in these areas.

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Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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