SYSTEMS ENGINEERING FOR SUSTAINABILITY IN A GLOBALIZED WORLD: RESOURCES, ECOSYSTEMS, BOUNDARIES

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Abstract

This paper discusses the role that the process systems engineering (PSE) community can play in addressing some of the challenges associated with sustainability in a globalized world. Through three case studies related to developing sustainable biofuels, synergistic design with ecosystems, and operating within an ecologically safe and socially just space, we offer insights into (1) how current PSE work has addressed problems in these and related areas; (2) what methodological challenges have to be overcome to address some key questions; and (3) promising research directions for PSE researchers and opportunities for expanding their boundaries, and accounting for resources and ecosystems.

Keywords

Sustainability; Renewable energy; Ecosystems; Social justice; System design, operation and control.

Introduction

Sustainability and globalization are both highly relevant to the chemical industry. They have affected previous developments and are expected to have an even larger effect on the future of the industry. Sustainability requires processes and products to be ecologically viable, socially desirable, and economically feasible for current and future generations. Globalization expands economic activities beyond regional and national boundaries through vast supply and demand networks, fast communications, and global movement of goods, services, and people.

The chemical industry is an important contributor and beneficiary of both trends. Its products are essential for meeting human needs, but they also contribute to ecological degradation by mobilizing fossil resources that contribute to global climate change and by introducing novel entities that can harm the environment and society. Sustainability is an urgent imperative and an existential threat to the chemical industry and humanity. In response, most corporations have pledged to achieve net-zero greenhouse gas emissions, wastes, and other environmental impacts within a few decades. The chemical industry has also been struggling economically as indicated by its decreasing contribution to global GDP, lower market valuation, and stagnant economic growth. The industry also contributes to social well-being by affecting employment, inequity, and health.

Globalization has allowed industry to benefit from economies of scale, mobility of the workforce, and efficiency of business networks. Its impact on the global economy is largely positive, at least in terms of gross domestic product. However, globalization can also make supply chains more fragile, as indicated by substantial disruptions due to events such as pandemics, war, and resource scarcities. There is also recent backlash against globalization as indicated by increasing tariffs against imported goods and national efforts toward self-sufficiency in many countries. Side-effects of globalization on increasing social inequities and environmental impacts are likely contributors to this backlash.

Sustainability and globalization present a large number of challenges and opportunities. Some that are specific to the PSE community include,

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a) *Renewable resources* need to be adopted for sustainability and for reducing reliance on globalization. This introduces challenges due to the intermittency of many renewable resources such as solar and wind. Other challenges associated with renewable resources include industrial heating, electrification, development of solar fuels, energy storage and hydrogen economy.
b) *Circular economy* aims to develop anthropogenic cycling of all molecules to minimize their environmental impact. This is essential for meeting corporate and national net-zero pledges, and may require nothing less than reinvention of the chemicals and materials industry toward greater decentralization, modularization, and shift of focus from manufacturing products to providing services. Relevant challenges include supply chain operation and control, reverse logistics, dealing with greater variability in recycled materials, balancing network efficiency with robustness, and circularity with sustainability.
c) *Nature-positive engineering* is needed to reverse the ecological decline that has been caused by human activities. This requires a shift in the engineering paradigm from ignoring or dominating nature to learning from nature and respecting it. This presents opportunities in all areas of PSE, but requires understanding the fundamental shortcomings of traditional engineering along with expansion of the system boundary to include regional and global ecosystems and services.
d) *Social equity* is increasingly relevant to business decisions but has mostly been excluded from the engineering system boundary. Recent insight into the ecologically safe and socially just space in regions across the world and the role of industrial activities and supply networks in expanding this space presents novel opportunities for PSE.

Meeting such challenges requires expansion of the PSE system boundary to include larger systems such as the economy, ecosystems, and society. Transdisciplinary or convergent collaboration is needed between disciplines. In the rest of this paper, we describe three case studies to offer insights into some of the above points.

Design and Operation of Integrated Biofuel Systems

We discuss lignocellulosic biofuel supply chains (SCs) as an example of a problem that (1) has a number of unique and new characteristics and therefore requires the development of new methods; and (2) requires the consideration of aspects not typically encountered in traditional PSE problems.

Background

Conventional manufacturing SCs, which have been studied extensively, have the following characteristics:

a) With the exception of oil refineries, where multiple crudes can be used, most SCs have defined sets of inputs (raw materials).
b) The inputs are of *fixed* and/or *known* quality, that is, they either have to meet strict specification or, if they do not, then their quality (and thus yields to intermediates and final products) is known.
c) The supply of raw materials comes from known point sources (e.g., known vendors, ports).

However, biofuels SCs are quite different:

a) An economically viable lignocellulosic fuel will have to process bioenergy crops of drastically different types (e.g., grasses and woody biomass).
b) Even for a given crop, the quality can vary significantly across suppliers and, most importantly, across years as changing environmental conditions (e.g., rainfall) significantly impact biomass content and digestibility.
c) Input sources are geographically distributed, that is, they are located in a region (area) rather than vendor facilities of ports (points).

Clearly, accounting for the above characteristics requires the development of new frameworks and methods, as described in the next subsections. It also requires the consideration of many aspects in addition to the ones considered in systems traditionally addressed in PSE (e.g., selection of biorefinery pretreatment and conversion technologies, consideration of carbon capture, consideration of technology and demand uncertainty). Interestingly, these new aspects, outlined below, require an integrated approach between design and operations:

a) *Land selection*. To avoid competition with food, it is recognized that bioenergy crops have to be established in what is termed *marginal* or *bioenergy lands*, that is, lands that are not and cannot be used for food (Gelfand et al., 2013). However, there are various definitions and categories of bioenergy lands, including low capability land, recently abandoned land, historically abandoned land, etc.
b) *Crop selection*. Different bioenergy crops (e.g., switchgrass, poplar, sorghum) have distinct advantages and disadvantages in terms of productivity (ton/acre), management methods and cost, types of suitable pretreatments, yields to fuels, etc. The trade-offs among these features are nontrivial and require the modeling of land, feedstock, and biorefinery operations.
c) *Land/crop management*. Fundamentally, management (e.g., irrigation, fertilization) can lead to higher productivity which, however, comes at a higher economic and environmental cost (e.g., cost and energy required to produce and transport fertilizers). In addition, the response of different combinations of land types and crops can be rather different and, importantly, geographically varying. Therefore, determining the optimal management is challenging.
d) *Uncertainty due to climate change*. Unlike most studied systems, and their corresponding uncertain parameters, the uncertainty in, for example, annual rainfall and temperature profiles, due to climate

change is limited. Most importantly, the impact of these uncertain profiles in the key parameters (e.g., crop productivity) is only now beginning to be, partially, quantified (Martinez-Feria and Basso, 2020). As if this was not sufficiently challenging, the impact of climate change in the availability of available lands/crop combinations is not well understood. For example, will a warmer climate expand, northbound, the region in which certain crops can grow?

Challenges and Opportunities

Since lignocellulosic biofuel systems have not been established yet, developing frameworks that would allow us to accurately calculate key environmental and economic outcomes can have an important impact. While PSE can play a key role in this development, the knowledge as well as nature and wealth of data that would be necessary mean that expertise from other disciplines would be of paramount importance.

To give one example, consider the land and crop decisions described above. First, it is important to recognize that the environmental impact of an integrated biofuel system depends, primarily, on the environmental performance of the land/crop subsystem and, secondarily, on the biorefinery subsystem. This is because the impact from, for example, carbon soil sequestration can be more important, and harder to quantify, than carbon emissions at the biorefinery. Second, since the available lands and suitable crops are region specific, the optimal biofuel SCs will also be region specific, employing different combinations of lands, crops, and biorefinery technologies. Thus, to truly understand these systems, we will have to use extensive geographic information, as well as data coming from plant and soil scientists. While a preliminary framework integrating land, feedstock, transportation and biorefinery considerations was recently proposed by O'Neil et al. (2022) (see Figure 1), the framework has to be extended to account, for example, for more environmental outcomes.

Second, the study of the lignocellulosic biofuel SCs requires the development of new methods in at least three areas:

a) *Spatially explicit models/approximations*. It was recently shown that considering land/feedstock decisions in a spatially explicit manner (e.g., 4x4 km cells) leads to SCs that are significantly better than the ones obtained when county-level information while, at the same time, biofuel SCs have to be designed at a regional level. Thus, the development of modeling and solutions approaches for spatially explicit regional biofuel SC models remains an open challenge.
b) *Surrogate models for crop productivity*. Crop productivity depends on biotic interactions in the soil, the weather, and management decisions. While relatively accurate *process* models are available to predict key outcomes in terms of these three types of inputs, the direct integration of these models with SC optimization models is intractable.
c) *Multi-period LCA approaches*. The environmental impact of these systems varies, significantly, with time. For example, carbon soil sequestration can be rather large the first few years after bioenergy crop establishment, but diminishes over time, whereas the benefits from ecosystem services is expected to increase over time. Thus, to accurately predict outcomes, (data for) new multi-period LCA methods are necessary.

While the development of methods to address the above challenges will enhance our understanding of the impacts of such systems, the key challenge remains the generation and use of realistic data coming from a range of disciplines. In that respect, PSE researchers can have a significant impact through collaborators in these other disciplines.

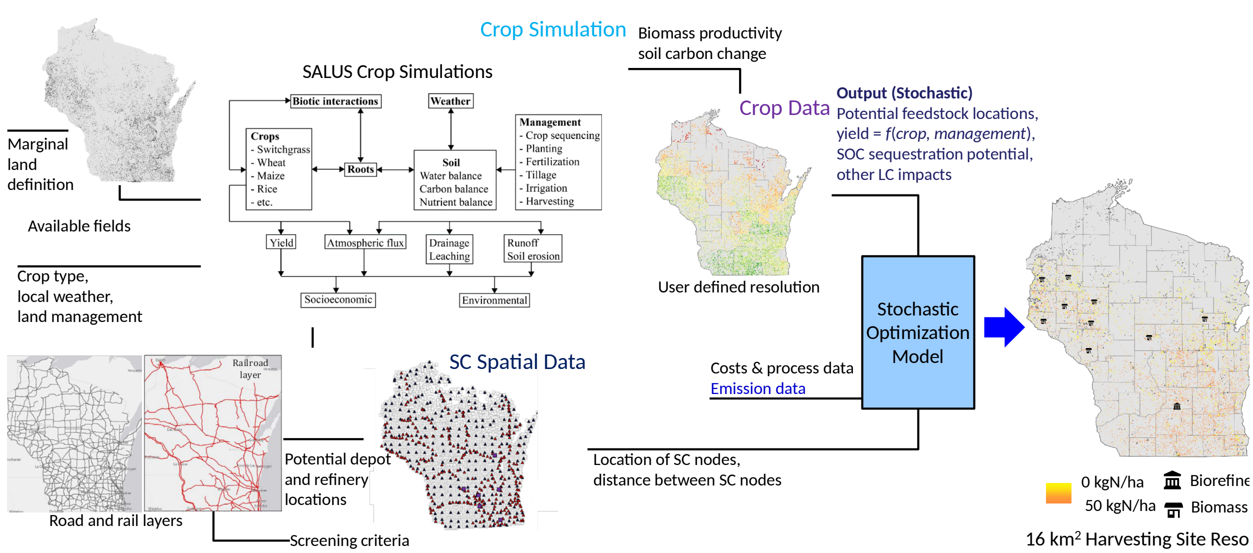

Figure 1: Graphic representation of framework of O'Neil et al. (2022).

Boundary Extensions

In the previous two subsections, we discussed what can be termed as the integrated landscape-feedstock-biorefinery problem. However, to truly understand the major drivers towards the development of a sustainable biofuel economy, the boundary of the system has to be expanded to include the following three areas:

a) *Biodiversity*. Current approaches to LCA do not quantify the benefits of ecosystem services and biodiversity in particular. In short, productivity and efficiency enhancements require mono-cultures of, typically, annual crops. It is however recognized that from an ecosystem services standpoint, perennial polycultures are beneficial (Robertson et al., 2017). Biodiversity depends not only on the spatial mixture of crops but also temporal considerations such as annual rotations and harvests per year. Unfortunately, existing LCA methods cannot quantify the environmental impact of biodiversity and thus underestimate the benefit of well-designed biofuel systems. Accordingly, the development of LCA methods that account for biodiversity is a fertile area of research.
b) *Policy and economics*. One of the challenges towards the development of a bioeconomy is the adoption of bioenergy crops by farmers. As is the case, interestingly, with process industries, farmers are not willing to change practices in the face of (economic and policy) uncertainty, which naturally leads to a number of interesting questions: *What policies and incentives would encourage farmers to change their rotations? What type of (long-term) contracts would be required to establish a resilient SC?* Designing these policies is outside the scope of PSE, but the integration of such biofuel-specific considerations in long-term planning models is important.
c) *Social Acceptance*. The penetration of renewable technologies is tightly interconnected with social acceptance. In that respect, incorporating research that uses, for example, dynamical systems and game-theoretical methods informed by empirical behavioral science to gain insights into how low-carbon energy transitions are impacted by societal norms, can be an interesting research avenue for PSE researchers (Constantino et al., 2021).

Manufacturing for Profit, Health, and Ecosystems

This example describes how chemical processes could be designed, operated and controlled to not only be profitable but to also benefit public health and respect nature's carrying capacity.

Background

Chemical processes are typically operated at specified set points to meet quality, safety and other technological and market requirements to maximize corporate profit. Direct interaction with the environment via resource use and emissions are considered for meeting regulations, and more recently, sustainability goals. However, most PSE efforts ignore, 1) whether local, regional, and global ecosystems have the capacity to supply goods and services that sustain the process, 2) the ability of ecosystems to complement technologies by removing pollutants and providing resources, 3) the impact of emissions on public health. The framework of techno-ecological synergy (TES) (Bakshi et al., 2015) seeks synergies between industrial and ecological systems to encourage engineering decisions that benefit from nature's "free" goods and services while respecting ecological carrying capacity to encourage ecological restoration instead of its degradation.

TES aims to shift the engineering paradigm from taking nature for granted and aiming to dominate it to a paradigm that explicitly accounts for the role of nature in sustaining engineering and human activities, learns from it, and respects its limits. TES expands the boundary of engineering to explicitly include nature's role and designs and operates industrial processes by including forests, wetlands and other ecosystems as unit operations. Just as a distillation column purifies product and recycle streams, trees and wetlands remove pollutants to provide clean air and water to industry and society.

Several designed TES systems, including manufacture of biodiesel and chlorine, and landscapes for renewable energy convey that the resulting innovative designs can be economically and ecologically superior to conventional engineering designs. However, like conventional process design, these TES designs are also based on steady-state models. For industry and society to truly reap benefits from TES systems, approaches are also needed for their operation and control. This presents many challenges due to fundamental differences between the dynamics of human-designed technological systems and self-designed ecological systems.

Challenges and Opportunities

Engineers prefer to design controllable systems that usually operate at set points. Such homeostasis is also found in natural systems, but only at the scale of an organism or smaller. At scales larger than an organism such as landscapes, societies, and populations, natural systems are homeorhetic. Such systems do not have a fixed set point but vary within a range of values. Imposing homeostasis on such systems has been a hallmark of many engineering activities. For example, dams impose homeostasis on the amount of water in a river, heating and cooling systems impose homeostasis on natural temperature fluctuations in the built environment. Such forced homeostasis contributes to human well-being and comfort, but it also results in erosion of system resilience, and makes human-designed systems less capable of recovering from large perturbations such as floods, droughts and heat waves, which are increasingly common.

With this insight, sustainability and resilience of TES systems requires that instead of imposing homeostasis on naturally homeorhetic systems, TES systems should be operated such that technological systems adapt to nature's intermittency. This presents many challenges and opportunities, as illustrated by recent integrated TES design and operation of a chlor-alkali process with a coal burning power plant to supply electricity, and a selective catalytic reactor (SCR) unit and local forest to mitigate NOx emissions (Shah and Bakshi, 2021).

Operation of such a system poses challenges due to the presence of phenomena over many temporal scales: from minutes to decades. The effect of meteorological conditions is felt over minutes, diurnal and seasonal variation over hours and months, and tree growth over decades. In the integrated design and control problem, size of the SCR and area of reforestation may be design variables, while quantity of chlorine produced can be a control variable that adapts to nature's homeorhesis. This requires the chlorine production rate to be intermittent and the plant even needs to be shutdown on bad ozone days.

Initial results under the assumption of perfect information compare the cost to company with the cost incurred by society due to the health impact of emissions. As compared to the conventional technology-only approach, which cannot find solutions with zero societal impact, the TES design and operation can eliminate societal impact by encourage ecological protection and restoration with only a small increase in the cost to company. TES design and operation is also less intermittent with fewer shutdowns as compared to the techno-centric solution.

Realizing the promise of such a TES design and operation needs methods to handle the complexity of ecosystem models and the highly intermittent spatio-temporal variation and multiscale character of ecosystems. Advances in approaches such as model-predictive control, Bayesian optimization, and surrogate modeling are needed for solving practical TES design and control problems.

Boundary Extensions

For the chemical industry to benefit from seeking synergies between industrial and ecological systems, PSE needs to expand its boundary to include ecological systems and their goods and services (Bakshi, 2023). The role of biodiversity and indigenous species in sustaining industry and society should also be included. Thus, rather than maximizing efficiency of a few ecosystem services, TES design and operation will need to integrate systems engineering with ecosystem restoration and systems ecology to account for a larger system. Aspects such as impact on public health also need to be included.

Ecologically Safe and Socially Just Supply Chains

In this section, we describe emerging approaches for quantifying the sustainability requirements of respecting ecological carrying capacity and of meeting basic human needs. We describe ways of operationalizing the "safe and just space" (SJS) with physical models and their potential use for designing global supply chains.

Background

For incorporating sustainability, the boundary of PSE has expanded from economic considerations to include life cycle environmental impact. Traditional life cycle assessment (LCA) aims to reduce environmental impact and is best suited for choosing the relatively better option. However, conventional LCA ignores the need to operate within nature's limits. Recent efforts are addressing this shortcoming by absolute environmental sustainability metrics that compare the demand and supply of specific ecosystem services. The demand is quantified by resource use and emissions, while the supply is based on ecological data and models. Many efforts also estimate the supply by downscaling "planetary boundaries" (Rockstrom et al., 2009) which are upper limits or "ecological ceiling" that must be respected in impact categories such as climate change, water use, land use, biodiversity loss, disruption of biogeochemical cycles etc. The space below this upper limit is called the "safe operating space" for humanity to thrive. Exceeding these limits increases the risk of irreversible damage to global ecological processes.

Sustainability is not just about the environment; human needs also need to be met. This requires adequate availability and use of goods and services from nature for human use. This minimum is the "social foundation" for sustainability. The region between the ecological ceiling and social foundation is the "safe and just space" (SJS) for humanity (Raworth, 2017). For human activities to be ecologically safe and socially just, their impact needs to be in the SJS. Satisfying this requirement is also an increasingly popular goal for industrial products, which makes it relevant to PSE.

Challenges and Opportunities

While the SJS is conceptually attractive, operationalizing it for making decisions is challenging due to the diversity of units representing ecological and social limits. For example, ecological boundaries are represented in physical units such as tons of CO_2 emitted and cubic meters of water available, while social aspects are represented as percentage of the population without access to clean water, sanitation, or education. Increasing the number of objectives is also undesirable.

Recent work shows how the SJS may be represented in terms of ecosystem services (ES) that are needed to meet basic needs of food, energy and water (FEW). Relevant flows and thresholds may be quantified in terms of ecosystem services such as carbon sequestration and water provisioning as follows,

- *Ecological ceiling* is determined by the capacity of local ecosystems to provide the selected ES. It is estimated by biophysical models or remote sensing.

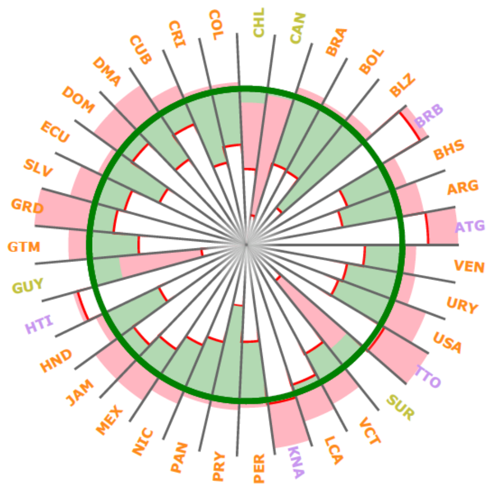

Figure 2. Safe and Just Space for meeting food-energy-water needs in the Americas and Caribbean. (Aleissa and Bakshi, 2022)

- *Social foundation* is the ES that must be used to meet minimum FEW needs of society. It may be derived from national and international databases.
- *Demand for ecosystem services* depends on human consumption and technologies used for meeting FEW needs such as power generation and farming.

Based on public domain data, these quantities for the carbon sequestration ecosystem service are calculated for 178 nations as shown for some in Figure 2. (Aleissa and Bakshi, 2022) Nations such as Chile, Panama and Brazil have a SJS as indicated by the green region, while others such as Haiti and Barbados do not. Among those with a SJS, only Chile, Canada, Guyana and Suriname are actually safe and just since emissions from their consumption (pink region) lie in the SJS (green region). Most nations, including the US, Brazil and Argentina are just but not safe since emissions from meeting FEW needs exceed the nations' capacity to sequester them (green line).

For corporations to operate in a manner that is ecologically safe and socially just, such data may be used to guide decisions related to operation of their facilities, location of new facilities, and selection of suppliers and users along their life cycle. For example, China and Bolivia are two sources of Lithium. Both have a SJS and both are just but not safe. Details such as the much larger SJS for Bolivia and the larger extent of overshoot for China may be used to favor Bolivia as the source of Li. Such information may be obtained for other ecosystem services as well, and become part of multiobjective optimization that is commonly used to guide decisions toward sustainability. Physical models of the SJS can also be used to identify approaches for bringing nations within their SJS or for creating a SJS if it does not exist. Such approaches may include switching to cleaner fuels to generate electricity, regenerative farming practices, and policies to encourage such a transition.

Boundary Extensions

Such work can benefit from expanding the boundary of conventional PSE to include aspects of social science such as ways of reducing societal inequities, geography to model global implications of safe and just decisions, and environmental economics and policy to determine appropriate incentives and policies for transitioning to safe and just supply chains and products.

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References

Aleissa, Y. M., Bakshi, B. R. (2022). Meeting national food-energy-water needs in an environmentally safe and socially just manner. *Technical Report*, The Ohio State University.

Bakshi, B. R. (ed) (2023). *Engineering and Ecosystems: Seeking Synergies toward a Nature-Positive World*, Springer.

Bakshi, B. R., Ziv, G., Lepech, M. D. (2015). Techno-Ecological Synergy: A Framework for Sustainable Engineering. *Env. Sci. Technol.*, 49, 3, 1752-1760.

Constantino S. M., Schlüter M., Weber E.U., Wijermans, N. (2021). Cognition and behavior in context: a framework and theories to explain natural resource use decisions in social-ecological systems. *Sustainability Science*, 16, 1651–1671.

Gelfand I., Sahajpal R., Zhang X., Izaurralde R.C., Gross K.L., Robertson G.P. Sustainable bioenergy production from marginal lands in the US Midwest. *Nature*, 493, 514-7.

Martinez-Feria R., Basso B. Predicting soil carbon changes in switchgrass grown on marginal lands under climate change and adaptation strategies. *GCB Bioenergy*, 12(9), 742-55.

O'Neil E.G, Martinez-Feria R.A., Basso B., Maravelias C.T. (2022). Integrated Spatially Explicit Landscape and Cellulosic Biofuel Supply Chain Optimization Under Biomass Yield Uncertainty. *Comp. Chem. Eng.*, 160, 107724.

Raworth K. (2017). A doughnut for the anthropocene: humanity's compass in the 21st century. *Lancet Planetary Health*, 1, e48-e49.

Robertson G.P., Hamilton S.K., Barham B.L., Dale B.E., Izaurralde C., Jackson R.D., Landis D.A., Swinton M.S., Thelen K.D., Tiedje J.M. (2017). Cellulosic Biofuel contributions to a sustainable energy future: Choices and outcomes, *Science*, 356, 1349.

Rockstrom J., et al. (2009). A safe operating space for humanity, *Nature*, 461, 472-475.

Shah U., Bakshi B. R. (2021). Toward nature-positive manufacturing by adapting industrial processes to pollution uptake by vegetation, *ACS Sust. Chem. Eng.*, 9, 49, 16709-16718.