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Toward Sustainable Chemical Engineering: The Role of Process Systems Engineering

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Abstract

Products from chemical engineering are essential for human well-being, but they also contribute to the degradation of ecosystem goods and services that are essential for sustaining all human activities. To contribute to sustainability, chemical engineering needs to address this paradox by developing chemical products and processes that meet the needs of present and future generations. Unintended harm of chemical engineering has usually appeared outside the discipline's traditional system boundary due to shifting of impacts across space, time, flows, or disciplines, and exceeding nature's capacity to supply goods and services. Being a subdiscipline of chemical engineering, process systems engineering (PSE) is best suited for ensuring that chemical engineering makes net positive contributions to sustainable development. This article reviews the role of PSE in the quest toward a sustainable chemical engineering. It focuses on advances in metrics, process design, product design, and process dynamics and control toward sustainability. Efforts toward contributing to this quest have already expanded the boundary of PSE to consider economic, environmental, and societal aspects of processes, products, and their life cycles. Future efforts need to account for the role of ecosystems in supporting industrial activities, and the effects of human behavior and markets on the environmental impacts of chemical products. Close interaction is needed between the reductionism of chemical engineering science and the holism of process systems engineering, along with a shift in the engineering paradigm from wanting to dominate nature to learning from it and respecting its limits.

1. WHAT MAKES CHEMICAL ENGINEERING UNSUSTAINABLE?

It is undeniable that chemical engineering has played an essential role in enhancing human well-being. Perhaps its greatest contribution is artificial fertilizers by means of the Haber-Bosch process, without which sustaining almost 7.5 billion people on the planet may have been impossible. Other key contributions include the harnessing of resources for providing consumer goods and transportation fuels; new types of materials for packaging, tissue engineering, and computing; innovations in medicines and medical devices; and countless others. Unfortunately, the direct and indirect impacts of many of these advances have contributed to the deterioration of ecosystems and their capacity to provide goods and services that are essential for sustaining human well-being. This paradox raises questions about the contribution of chemical engineering to sustainable development. In particular, the chemical industry has helped mobilize billions of tons of fossil resources that are major contributors to the accumulation of greenhouse gases in the atmosphere and the resulting global climate change. Artificial fertilizers also contribute to the emission of greenhouse gases due to the nitrous oxide emitted after the application of nitrogen fertilizers and the carbon dioxide emitted after using hydrogen from methane for producing ammonia. Nitrogen and phosphorus fertilizers are also implicated in the formation of aquatic dead zones across the planet due to harmful algal blooms that feed on fertilizer runoff. Despite their many unique and seemingly irreplaceable properties, plastics are now being banned in many parts of the world due to their contribution to solid waste accumulation on land and in the oceans. These are among many examples of unsustainable chemical engineering: Even though chemical engineering products and processes meet the needs of the present, many products are compromising the ability of future generations to meet their own needs. Thus, the side effects of many chemical products and processes violate the classic definition of sustainable development (1).

Such negative side-effects are invariably unintended and unexpected. However, given that the consequences of unsustainable products and processes violate engineering's goal of "solving problems for people and society" (2), reducing the chance of unsustainable products and processes is among the most important challenges facing the field today.

The common response of engineering to such problems has been to develop more and better technologies. For example, once the role of chlorofluorocarbons in stratospheric ozone depletion was accepted, alternatives were developed that had a smaller ozone depletion potential. Similarly, to address the problems associated with ammonia-based fertilizers, methods are being developed for decentralized ammonia manufacture and precision farming. New types of degradable plastics are less likely to accumulate in the environment. To address the emissions of greenhouse gases, methods for carbon capture, utilization, and storage are being developed. Renewable energy systems are also considered to be sustainable, and many efforts are focusing on energy storage and smart power grids. Will these and other technological advances ensure that chemical engineering does not degrade ecosystems and guarantee their availability for the well-being of future generations?

A close look at environmentally and societally unacceptable outcomes from engineering indicates that the unintended harm almost always appears outside the system boundary of engineering (3). Traditionally, the boundary of chemical engineering has included the product, its manufacturing, its raw materials, and its supply chain. Environmental systems like the stratosphere where the ozone hole appeared, the global climate that is disrupted by accumulation of greenhouse gases, ocean gyres where plastic islands form, and lakes and oceans that suffer harmful algal blooms were not within the system boundary of the engineering that developed these products.

Newer refrigerants such as hydrofluorocarbons have a small ozone depletion potential but a high global warming potential. Thus, this alternative technology shifts the environmental impact

from one type of emission and impact category to another. Electric cars having zero emissions does not imply that they have zero environmental impact. This is because the emissions may shift from the car's tailpipe to the smokestack of the electricity producer and the materials needed for energy storage. Engineering also focuses on improving technological efficiency per unit of product (such as energy use per liter of desalinated water), yield of desired product, and efficiency of fuel combustion. Such advances do result in less use of resources and lower emissions per unit of product, and engineers commonly assume that these benefits will transfer to society when the products are used at a larger scale. Unfortunately, this intensive view of scientific innovation and technology development fails to consider the effect of large-scale adoption of the technology when the unintended harm can shift across disciplines. For example, a more efficient device is usually less expensive in terms of the cost per unit of service provided. This encourages consumption in the economy and increases impact, reducing or even nullifying any benefits per unit of product. This "rebound effect" shifts the impact from the domain of engineering to that of human behavior and economics (4, 5).

Thus, if chemical engineering is to develop sustainable solutions, it needs to reduce the chance of such shifts by expanding its system boundary. In addition, since impacts appear in environmental systems, the impact of engineering activities on these systems and the capacity of these systems to absorb the impact also need to be considered.

Based on such insight, it is clear that unintended environmental harm from engineering decisions, and therefore unsustainable engineering, can occur due to the shifting of impacts across space, time, disciplines, or flows. Furthermore, environmental harm occurs when the activities exceed nature's capacity to absorb emissions and mitigate their impact or to provide resources without depletion of the stocks. This understanding points toward six necessary but not sufficient requirements that need to be satisfied before claiming environmental sustainability (6). Methods need to account for shifting of impacts in four spheres: space, time, across disciplines, and between flows. In addition to these four requirements, methods also need to account for the demand of ecosystem services created by emissions and resource use, and the capacity of relevant ecosystems to supply these demanded goods and services.

In addition to being environmentally sustainable, products and processes also need to be economically and societally sustainable. Due to the complex interactions between environmental, economic, and societal systems, sustainable development belongs to the category of "wicked" problems (7–9). These problems are difficult to solve since it is not possible to even formulate them in an unambiguous manner while capturing all the requirements. The complexity of such problems means that it may not be possible to find the "correct" answer, but only to know whether a decision is better or worse.

Motivated by these challenges for ensuring chemical engineering's positive contributions to sustainable development, this article focuses on the role of process systems engineering (PSE) in ensuring a sustainable chemical engineering. It provides a critical review of how PSE has been working toward this goal and builds upon previous reviews (10, 11) and perspectives (3, 12). The next section provides an overview of the role and evolution of PSE, and the influence of the quest toward sustainability on its recent development. This is followed by a critical review of advances in PSE in four areas of research activity: metrics for quantifying sustainability of industrial processes, design of chemical processes and their supply chains, design of single- and multimolecular products and their formulations, and dynamics and control of chemical processes. The last section describes some of the challenges that remain and potential barriers to overcoming them.
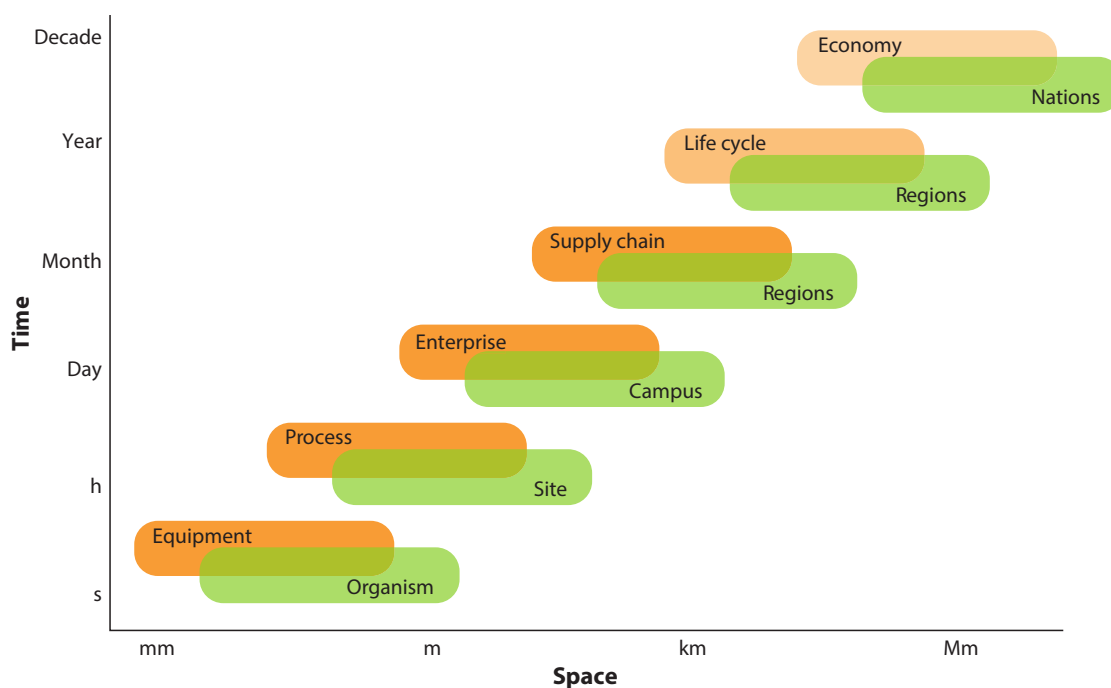
Figure 1

Systems relevant to sustainable chemical engineering. From the scale of individual equipment, process systems engineering has gradually expanded over the last few decades to consider the process, enterprise, and supply chain (*dark orange ovals*). Sustainability requires further expansion to consider the life cycle and economy (*light orange ovals*). The dependence of industrial activities on goods and services from nature needs to be considered at all scales, ranging from individual equipment to processes, life cycles, and the economy (*green ovals*).

2. ROLE OF PSE IN THE QUEST FOR SUSTAINABILITY

Most research in chemical engineering adopts a reductionist view. This approach excels at developing new scientific insight and advancing it toward practice. Such work results in developments such as new and improved catalysts, separation processes, biomedical devices, and materials, but its narrow view makes it prone to the shifting of environmental impacts and unintended harm. It lacks the type of systems or holistic view that is needed to reduce the chance of shifts and unintended harm described in Section 1. The subdiscipline of chemical engineering that is most capable of developing the needed holistic view is PSE.

Traditionally, the focus of PSE has been on the economic feasibility of chemical process systems. From the scale of individual equipment, PSE has gradually expanded over the last few decades to consider the process, enterprise, and supply chain (**Figure 1**) (13, 14). This has resulted in methods for process design, enterprise-wide management, and supply chain design. PSE has also expanded to consider smaller scales such as systems of particles, molecules, and atoms, and these efforts have resulted in methods for molecular design. In addition to the goal of improving profitability of the chemical industry, environment, health, and safety have also appeared as objectives or constraints.

Until the 1980s, industry mostly ignored or even denied its impact on the environment (15), as shown in the left part of **Figure 2a**. One exception was the development of methods for reducing energy use, which were motivated by the oil crisis of the 1970s. As restrictions on what chemical processes could emit became tighter, industry was forced to find ways of satisfying these limits while maintaining profits. This resulted in methods that included the local environment as a

Approach	Optimization problem formulation
a **Ignore the environment** Maximize profit	max $P(x_{eq})$ Subject to $F(x_{eq}) \geq 0$
b **Environment as a constraint** Maximize profit Satisfy environmental constraints	max $P(x_{eq})$ Subject to $F(x_{eq}) \geq 0$; $D(x_{eq}) \leq 0$
c **Local impact as an objective** Maximize profit Minimize local environmental impact	max $P(x_{eq})$; min $D(x_{eq})$ Subject to $F(x_{eq}) \geq 0$
d **Life cycle impact as an objective** Maximize profit Minimize life cycle environmental impact	max $P(x_{eq})$; min $D(x_{eq}, x_{vc})$ Subject to $F(x_{eq}) \geq 0$; $L(x_{eq}, x_{vc}) \geq 0$
e **Respecting nature's capacity as objective** Maximize profit Minimize overshoot of ecosystem services	max $P(x_{eq})$; min $V(x_{eq}, x_{vc}, x_{el})$ Subject to $F(x_{eq}) \geq 0$; $L(x_{eq}, x_{vc}) \geq 0$; $E_{el}(x_{eq}, x_{vc}, x_{el}) \geq 0$
f **Accounting for markets and human behavior** Maximize private and social profits Minimize overshoot	max $P(x_{eq})$; min $V(x_{eq}, x_{vc}, x_{el})$; max $G(x_{eq}, x_{vc}, x_{el}, x_{en})$ Subject to $F(x_{eq}) \geq 0$; $L(x_{eq}, x_{vc}) \geq 0$; $E_{el}(x_{eq}, x_{vc}, x_{el}) \geq 0$; $E_{en}(x_{eq}, x_{vc}, x_{el}, x_{en}) \geq 0$

Figure 2

Stages of evolution of chemical engineering toward sustainability and formulation of the corresponding optimization problems. Abbreviations: D, environmental impact (demand for ecosystem services); E_{el}, ecological model; E_{en}, economic model; F, process model; G, gross domestic product; L, life cycle assessment model; P, profit; V, ecological overshoot.

constraint, while keeping profit maximization as the primary objective, as shown in **Figure 2b**. Gradually, environmental impact became part of the objective, since it often resulted in more innovative solutions that were "win-win": better for the environment and for profit. Initially, the focus was on minimizing local impacts caused directly by the process, as shown in **Figure 2c**. Realization of the shifting of impacts to other processes in the life cycle resulted in expansion of the boundary of PSE to include the life cycle, as shown in **Figure 1**, and efforts to minimize this
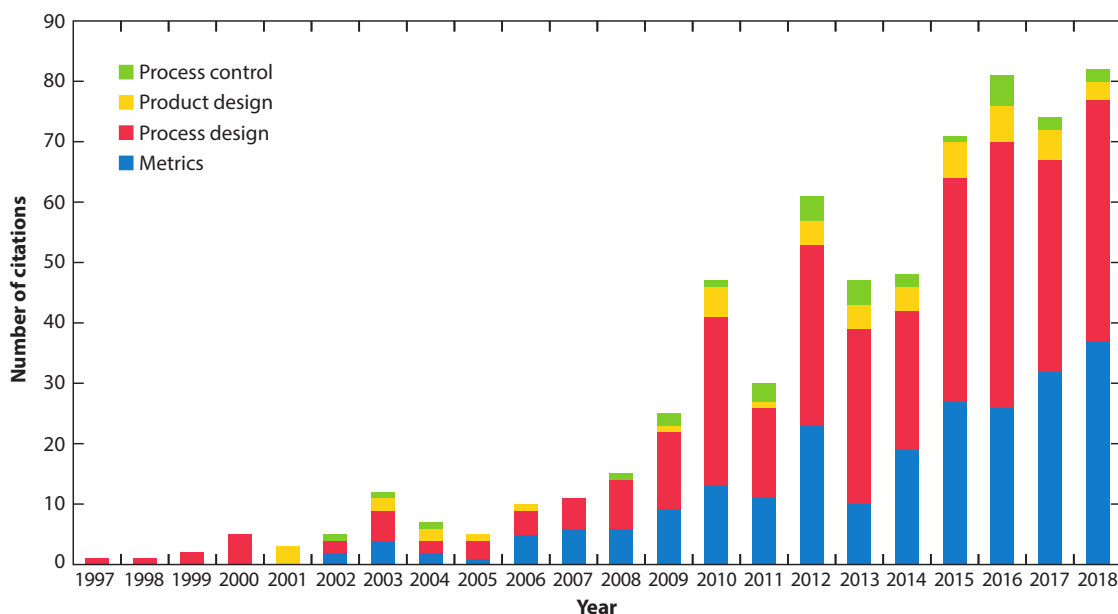
Figure 3

Publications that match keywords "sustainab*" and each of "process control," "product design," "process design," and "metrics"; the search was refined for the subject "Engineering, Chemical." Data are from Web of Science, accessed on September 11, 2018.

life cycle impact, as shown in **Figure 2d**. These efforts focus mainly on reducing the chance of shifting environmental impacts in space and between types of flows (resource inputs and environmental impacts). To account for nature's capacity to provide resources and mitigate the impact of emissions, PSE is starting to explicitly account for the dependence of industrial activities on goods and services from nature. This needs to be considered at all scales, ranging from individual equipment to processes, life cycles, and the economy. This expansion of PSE is indicated in **Figure 2e** and by the green ovals in **Figure 1**. Efforts are also being directed toward accounting for the impact of markets, human behavior, and societal aspects as depicted in **Figure 2f**.

3. ADVANCES IN PSE FOR ENABLING SUSTAINABILITY

Figure 3 shows the results of a literature search with keywords "sustainab*" and each of "process control," "product design," "process design," and "metrics," within the field of "Engineering, Chemical." The first papers related to sustainability and PSE appeared about two decades ago—a decade after the term "sustainable development" was introduced (1) at the Earth Summit. Early efforts focused on sustainable process design, which has been the most active area of research. The second most active area is related to defining metrics to determine the sustainability of chemical processes and products. Sustainable product design and process control have received relatively little attention. This section describes some of the main developments in these four areas of research.

3.1. Metrics

Supporting decisions that ensure positive contributions toward sustainable development requires metrics for quantifying sustainability. Ideally, such metrics need to be well defined, be easy to calculate and use for supporting decisions, and capture the requirements for claiming sustainability that were summarized in Section 1.
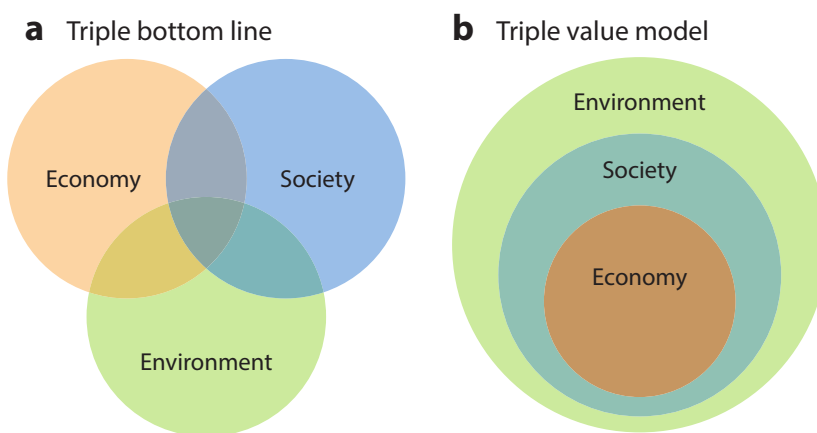
a Triple bottom line

Economy · Society · Environment

b Triple value model

Environment · Society · Economy

Figure 4

Views of sustainability. Economic, societal, and environmental systems are not independent with limited overlap (17), as depicted by the triple bottom line (*a*), but are nested systems (26), as depicted by the triple value model (*b*).

A popular understanding of sustainability in the context of engineering decisions is conveyed by the "triple bottom line" (16). This highlights the importance of economic, environmental, and social aspects of sustainability, and is often represented as shown in **Figure 4*a***. This understanding has resulted in many metrics for assessing sustainability that are classified as one-, two-, and three-dimensional depending on whether the metric covers only one, two, or all of the three bottom lines (17, 18). In terms of **Figure 4*a***, three-dimensional metrics are at the intersection of all three bottom lines while two-dimensional metrics are located at the intersection of any two bottom lines. Such a view has also been adopted by organizations such as the American Institute of Chemical Engineers (19, 20) and the UK Institution of Chemical Engineering (21). These metrics include indicators of sustainability innovation, environmental impact, safety, product stewardship, social responsibility, and value-chain management. Many of these indicators are subjective with a boundary that need not consider the full life cycle. Some corporations have also developed their own indicator systems (22, 23). Many metrics quantify eco-efficiency, which is the environmental impact from the process, product, or life cycle normalized by a quantity such as quantity produced or profit. A recent tool developed by the US Environmental Protection Agency, GREENSCOPE (24) is proposed to evaluate a reaction or process for sustainability by determining metrics relevant to the environment, energy, efficiency, and economics. It consists of approximately 140 indicators. Various methods have been devised to process such data and metrics to support decisions (25).

Selecting the most important metrics based only on greenhouse gases or water use is a popular approach, but it may result in loss of important information and shifting of impacts to other resource or emission flows. To reduce the chance of burden shifting in space along the supply and demand networks and between different types of flows, the approach of life cycle assessment (LCA) has been popular. This approach aims to consider all activities related to a selected product or process, "from cradle to grave." A major challenge in LCA is in obtaining data for the large and complicated life cycle network of most activities. Over the last two decades, this approach has been standardized, and software and databases have made it relatively easy to apply this approach. Most databases consist of facility-level data that are based on aggregation of multiple manufacturing processes from a selected region. Approaches for developing inventory data based on process models have also been proposed and are particularly well suited for emerging technologies and individual process units (27–30). Approaches have been developed for improving the quality of

life cycle inventory data by data reconciliation (31). Inventory data are available at the economy scale as environmentally extended input-output models (32).

A typical LCA results in a large amount of data that represents all the resources and emissions from the selected life cycle. Methods for aggregating such results are developed for life cycle impact assessment. This approach represents resource use and emissions in terms of several midpoint indicators such as global warming potential, eutrophication potential, and human toxicity potential (33). Methods have also been developed for further aggregation into single indicators for each area of protection, such as environmental impact, human impact, and resource depletion. Obtaining a single indicator of environmental impact may rely on ecological models of the relevant region. For determining human impact, methods used by the World Health Organization that quantify human impact in terms of years of life lost and years lived disabled may be used. Aggregating resource use can rely on scarcity information on each resource, or thermodynamic methods based on exergy analysis. Further aggregation of these three categories into a single indicator requires human valuation, and various standardized methods are available (33, 34).

Frameworks consisting of a hierarchy of indicators quantify impacts for individual processes or products at the equipment scale, their life cycle constructed by selecting the most important processes at the value chain scale, use of economic input-output models to capture flows at the economy scale, and even goods and services from nature at the ecosystems scale. A hierarchy of metrics may be calculated using exergy analysis (35). Such a hierarchy is also used in the framework of GREENSCOPE (36). Statistical methods have also been used for dimensionality reduction of sustainability metrics (37).

If the flows can be represented in terms of a common unit, then they may be combined to a single value. Exergy analysis is able to represent flows in terms of their capacity to do work (38, 39). Even the impact of emissions may be represented in terms of lost capacity to do work (40). Emergy analysis goes a step further and accounts for the contribution of nature by representing all flows in solar equivalent joules (40, 41).

Aggregate metrics may also be obtained by converting all quantities into monetary values. This aggregation includes market and nonmarket goods. Market goods have a price; they are things that money can buy. Nonmarket goods are intangibles such as the impact of emissions, depletion of resources, changes in social equity, justice, etc.

Eco-profit (42) and sustainability net present value (43) are recent metrics that have been used for solving various process design tasks. Such approaches have a long history in environmental economics, with inclusive wealth being a recent development (44). These metrics are convenient, since most people can relate to monetary values. However, methods for monetization of non-market goods and services can be highly controversial. Such metrics are said to quantify weak sustainability, as explained in more detail later in this section.

The methods described so far focus only on environmental sustainability, which may result in burden shifting to societal and economic impacts. The approach of life cycle sustainability analysis (45) considers environmental, economic, and social aspects by combining conventional or environmental LCA with life cycle cost (LCC) analysis and social LCA (sLCA). LCC accounts for monetary costs incurred in each step of the life cycle, while sLCA considers societal impacts such as reliance on child labor, unemployment, and quality of life.

For industrial processes, economic aspects are often captured by the net present value or another such monetary metric at the equipment scale by only considering the process that is of corporate interest. The LCC is often not considered. Getting data for sLCA is challenging, and for PSE applications, it is common to focus on the safety and job creation aspects of the process. Environmental aspects are often considered for the life cycle. For understanding the trade-offs between these triple bottom lines, they have been represented as vectors in the three-dimensional

environmental-economic-societal space to gain graphical insight into the sustainability space and to identify opportunities for improvement (46). Multi-criteria decision making has also been used to combine the three categories by relying on subjective weights (47), or by using approaches such as the analytic hierarchy process and its variations and extensions along with fuzzy representation to capture lack of precision. Such methods have been used to combine results from environmental analysis (48–50) and from life cycle sustainability assessment (51, 52). Some corporations have developed metrics tailored to their products and priorities (53, 54).

Despite the large literature and popularity of the sustainability metrics discussed so far, they do not satisfy all the requirements described in Section 1 for claiming sustainability. First, aggregation may result in implicit assumption of substitutability between indicators. For example, combining human impact, global warming, and water use into one metric implies that the three impacts are substitutable. That is, as far as the aggregated indicator is concerned, it does not matter which impact is reduced. Such an approach can only provide weak sustainability (55). Second, the concept of a triple bottom line, which has been the basis for most sustainability metrics, can be misleading for assessing sustainability. This is because it implies equal importance of economic, societal, and environmental aspects, but in practice, these are not equal. Economic, societal, and environmental systems are not independent with limited overlap, as depicted in **Figure 4a**, but are nested systems. Among the three, the one that is most important is the environment, since it provides the foundation to the other two systems. Without goods and services such as water, soil, pollination, and flood regulation, society cannot function. Without these ecosystem goods and services and without societal goods and services such as educational institutions, a legal system, and cultural norms, economic goods and services such as manufactured materials, markets, and trade cannot be produced. Thus, these three systems may be depicted as shown in **Figure 4b**, which has been called the triple value model (26). This implies that for sustainability, there is one foundational bottom line: the environment. The third shortcoming of existing metrics is that sustainability is about staying within nature's capacity, which is not considered. In terms of **Figure 2**, most current metrics do not go beyond **Figure 2d**.

Some metrics have been developed for addressing these challenges but have found limited use to date. They include the sustainability process index (56), which quantifies the degree to which local activities exceed assimilation capacities of the local environment. This capacity is defined according to local regulations. This metric converts all flows into land area to allow aggregation and comparison with nature's assimilation capacity or local environmental regulations. Further extensions have applied such approaches to individual processes and products (57, 58). This approach is related to the ecological footprint (59), which has been applied mainly at the national scale and focuses mostly on the land area needed to sequester CO_2 emissions, along with other direct uses of land for activities like farming.

The concept of planetary boundaries (60) identifies the limits of nature's capacity for some human impacts at the global scale. Efforts to downscale these boundaries to a region or process rely on subjective allocation between multiple activities (61). Metrics based on comparing the demand and supply of ecosystem services at local and regional scales have been suggested by using ecological models or data to quantify their capacity to provide various services (62, 63). The demand may be determined by the quantity of natural resources used and emissions, while the supply depends on the nature of local ecosystems. Unlike most other metrics, these metrics indicate absolute environmental sustainability, since they go beyond just comparing alternatives and actually account for the extent to which the selected activity exceeds nature's capacity (64). Such metrics also explicitly include the role of nature, and are closer to the common definitions of sustainability (1).

Most of the metrics for assessing sustainability implicitly assume that the system is static. Exceptions include the use of information theory metrics such as Fisher information, which are applied to a time series of data and are useful for predicting loss of resilience in complex systems (65).

3.2. Process and Supply Chain Design

These design problems may be formulated as optimization problems, and their evolution toward accounting for sustainability is shown on the right side of **Figure 2**. As shown in **Figure 2a**, the traditional approach for process design focused only on maximizing profit (P) subject to physico-chemical constraints of the designed flowsheet (F) with decision variables representing parameters in the equipment (x_{eq}). With increasing awareness about environmental impact, end-of-pipe treatment technologies were introduced to satisfy regulations. Models of these technologies are indicated in **Figure 2b** as $D(x_{eq})$, with D indicating the demand of ecosystem services quantified by resource use and emissions.

Such systems were found to be less cost-effective than designing or retrofitting processes to produce less waste (66), thus prompting work on new methods of designing and modifying processes with both economic and environmental considerations (67, 68). Many of the first efforts at environmental process design focused on (*a*) process integration to recycle chemicals and waste (69, 70) and (*b*) methods of quantifying a process's environmental impact and of incorporating that impact into the design process (71). Pinch analysis combined with process optimization allows processes to be designed from scratch with minimum energy and/or water consumption, leading to both environmental and economic benefits (72–74). However, it does not account for emissions and their environmental impact.

The waste reduction (WAR) algorithm was the first method of environmental process design to introduce the idea of accounting for upstream processes in the environmental impacts of the primary process. It is an iterative method for locating a process design with acceptable economics and minimum waste production. Waste production is quantified through the pollution index, defined as the mass of waste or pollution a process produces per mass of useful product (71, 75). Any chemical that is not consumed within a process or part of the final product is considered to be pollution. However, at first, only material flows were assigned a pollution index; energy flows were not included in the WAR algorithm. Upstream processes were accounted for through the pollution index of process inputs and raw materials. Subsequent refinements of the WAR algorithm included its integration with chemical process simulators to streamline the process (76), inclusion of environmental impact assessment (77, 78), and inclusion of energy flows (79).

Alternatives to the WAR algorithm generally involved evaluating several different options for a process—either materials or technologies—and choosing the most economical and least polluting option. In particular, the material intensity per service unit (MIPS) indicator was proposed as a tool to evaluate alternate technologies (80, 81). MIPS was seen as a less data-intensive alternative to LCA, suitable to early design stages when it may be difficult to obtain accurate life cycle inventory data. However, MIPS for the primary product and for emissions produced is defined as zero; thus, MIPS does not account for any emissions released to the environment. Similar work included a method for determining the cheapest legal treatment paths for waste (82) and a method using Eco-Indicator 99 to choose environmentally friendly process materials (83).

These approaches either were designed to minimize environmental impact or included the environment in the design problem as a constraint, as shown in **Figure 2b**. Developing a design that minimized impact was not likely to be practical because it might not be economically feasible, and imposing environmental considerations as a constraint meant that the design solution could not be

better than this constraint, which could stifle environmentally superior innovations. Such insight led to the inclusion of the environment as an objective along with the economic objective, as shown in **Figure 2c** (10, 84). Early work in this area focused on complexes of petrochemical processes, with the environmental objectives including energy and feedstock utilization (85) and toxicity reduction (86, 87). Optimization of utility systems and waste management systems followed (88, 89). Complete processes and supply chains were the last to be optimized under environmental objectives, with methodologies that frequently included pinch analysis or another form of process integration (73, 90–92). Additional work was done on ways of incorporating environmental criteria in early design stages (93) as well as in the final, more detailed stages.

Recognition of the problem of burden shifting resulted in expansion of the process design boundary to include the life cycle. Early work in this direction did not consider the full life cycle but only the important upstream processes that were responsible for most of the emissions. In particular, minimum-emission utility systems were designed by considering emissions from power-generating processes that supply the primary process (88); minimum-cost waste treatment systems were designed while including environmental impact from the treatment system and any remaining emissions (82). The concept of "optimal abatement," or a point at which more stringent waste treatment begins to increase total environmental impacts due to the extra energy and equipment required, was present in References 94 and 95. This tendency points to the beginnings of a systems perspective, in which chemical processes are acknowledged to have impacts outside the conventional design problem boundary (12).

LCA was brought into process design as a way to quantify the emissions of a process itself as well as the emissions caused by the process. Under waste minimization and single-process integration, it was possible to minimize impacts of a single process while creating extra impacts in connected processes (86, 96). Using LCA allowed these connected processes to be included in the design problem, resulting in process designs with lower overall impacts. The optimization problem formulation shown in **Figure 2d** includes the life cycle impact of resource use and emissions, D, which is a function of the equipment parameters, x_{eq}, and life cycle network parameters, x_{vc}, at the scale of the value chain. This has been called the life cycle optimization framework (94, 97). Early work on combining LCA with process design was an extension of the WAR algorithm (94, 98). Other early studies set the template for virtually all future work in this area (99, 100). Most use of LCA in process design has selected processes that are considered to be most important. The use phase of the product is also usually excluded, making the life cycle network almost identical to the supply chain (101, 102). Also, the focus has tended to be on one primary environmental impact such as carbon footprint (103–106), or a univariate aggregate indicator obtained by an end-point life cycle impact assessment method such as Eco-Indicator 99 (105–108). These methods that were used to combine LCA with process design were extended to supply chain design (97, 109–111).

Most of these efforts treat life cycle processes as linearly scalable "black boxes," and any interaction effects between the life cycle processes and the primary process are ignored (112). Such interactions could be due to the designed process and its by-products causing changes in the life cycle flows. For example, the by-products, like electricity from bagasse, may displace alternatives like conventional electricity from the grid. As the primary process is optimized and implemented, it will place more and/or different demands on its life cycle processes, causing those processes in turn to be redesigned and optimized to meet the new demand in a cost-effective and environmentally sound manner. In addition, most efforts consider only the value chain scale of the life cycle, which could result in burden shifting due to ignorance of flows in the processes excluded from the system boundary. Such disadvantages are expected to be most relevant to large-scale optimization problems at national scales, as demonstrated in Reference 111.

Some studies have accounted for the interaction between the designed process and its life cycle (113–116). Process-to-planet is a systematic framework for integrating models at the equipment, value chain, and economy scales (117). Models at the equipment scale are process models based on the underlying physicochemical phenomena, value chain models are linear empirical models of the partial life cycle, and economy scale models represent the economy of the selected region. The process-to-planet framework addresses some of the challenges identified in multiscale systems engineering for energy and the environment (118).

Recent work on sustainable design includes the use of multiple, often conflicting, environmental objectives like those described in Section 3.1 (119–123) and societal objectives such as job creation and safety (119, 124–127). Advances in optimization methods are also being used to quantify the trade-off between multiple objectives in the form of a Pareto surface. Further assessment can help in choosing a specific solution from this surface (128, 129) and lead to insight analogous to heuristics for sustainable design (130). Approaches have also been developed to account for uncertainties in single- and multi-objective optimization design problems (131–133).

Efforts in process design are also directed toward including the goal of respecting nature's limits, as shown in **Figure 2e**. This involves explicitly accounting for the role of ecosystems in supporting the relevant activities. The corresponding optimization problem formulation in **Figure 2e** includes ecological overshoot (V) as an objective, along with decision variables pertaining to ecological systems (x_{el}). Ecological overshoot may be determined by comparing the demand and supply of a selected ecosystem service, as described near the end of Section 3.1. At the equipment scale, ecosystems are being included as unit operations in process design (134) and regional systems (135, 136). Similarly, ecosystems are also included in supply chains (137, 138) and life cycles (64). A framework for developing techno-ecological synergies at multiple scales has also been developed (63). These efforts could enable an engineering that respects ecological constraints (139) and establishes mutually beneficial synergies with nature so that both technological and ecological systems can flourish.

Markets and human behavior play a critical role in determining whether engineering decisions contribute to sustainable development. The problem formulation for including these aspects is shown in the right side of **Figure 2f**. Here, the objective G represents a macroeconomic objective such as the gross domestic product, and E_{en} is the model of the economy, with decision variables x_{en}. The model of the economic systems is meant to capture the interaction between various economic sectors due to engineering decisions and the effect of human preferences. Such issues are considered in the approach of consequential LCA (140), which aims to account for the effect of new technologies on substitution of alternatives in the marketplace. Such an approach may be combined with the design of a process or its life cycle (141). The effect of markets on the cost of raw materials and their further effect on the feasibility of biofuels have been considered by connecting process design with a partial equilibrium model of the forest products economy (142). A multiscale model of the process, life cycle, and economy can help in considering the effect of the macroeconomy on specific manufacturing processes or products. Such an approach can account for practical limits such as availability of resources and emissions constraints, and their effect on corporate profits, life cycle impacts, and macroeconomic goals such as the gross domestic product. Including the effect of human behavior requires inclusion of information about price elasticity (143). This could benefit from the use of models that capture market equilibrium.

An industrial ecosystem is a network of manufacturing processes in which "the effluents of one process…serve as the raw material for another process" (144, p. 166). Such systems aim to mimic natural ecosystems to become sustainable just like ecosystems. Such mimicry is considered to be a promising way of addressing the wicked problem of sustainable development. The concept of such a system is process integration at the interprocess scale rather than the intraprocess scale used in

conventional pinch analysis. Connecting processes through material and energy flows allows for less waste, fewer environmental impacts associated with raw material extraction, and lowered costs for all participating processes (145, 146). Approaches for designing such networks have relied on extending the methods of PSE (147), such as the design of heat exchanger networks (148), the design of water networks to address goals of water quality and quantity (149–151), the optimization of materials use (152), and the design of equipment and flowsheets (153, 154). The effect of industrial symbiosis on network resilience is far from clear. Greater networking can make the network susceptible to cascading failures, or make it more resilient due to availability of alternate paths for raw materials and products. Metrics have been proposed for quantifying network resilience (155–157) and for guiding the development of industrial networks. Other efforts account for the surroundings in which the activities are located, such as watersheds (158). Numerous studies focus on reducing environmental impact, but multi-objective studies that consider economic and environmental aspects are also an active area of research (159).

Given the importance of food, energy, and water (FEW) for human well-being, and the interaction between their flows, many efforts are including this FEW nexus in several PSE tasks (160). Many PSE approaches have been used for understanding and designing systems while accounting for this nexus. Applications include agricultural, biofuel, urban, shale gas, and water distribution systems (160–162).

3.3. Product Design

Designing chemical products while accounting for sustainability considerations is a recent activity, as conveyed by the relatively small number of publications in **Figure 3**. A recent review identifies two types of products that are usually designed by chemical engineers (163). Single-species products include small molecules such as solvents and refrigerants, and large molecules such as surfactants and membranes. Multi-species products may be formulated, such as blended fuels, or functional, such as detergents and medicines. Finally, there are devices such as batteries and microcapsules. Sustainability is relevant to all types of products. As discussed in Section 1, the history of chemical products includes many that were unsustainable and have been banned. In many cases such as chlorofluorocarbons, the unsustainable characteristics and large environmental impacts became apparent only upon large-scale adoption. Methods for sustainable product design need to avoid such situations. In addition, methods are also needed to incorporate sustainability at early stages of design, when data may be scarce. This is because by the time better data become available, it may be too late to modify the design.

For the design of single-species molecules such as products from biomass, the approach of reaction network flux analysis has been extended to include economic and environmental considerations. Such an approach has been used to choose the reaction pathway for making biofuels and biochemicals from glucose (164) and polymers from biomass (165). At this early stage of decision making, environmental considerations are often approximated by the heat of reaction and the life cycle impact of raw materials needed for each pathway. Economic aspects are approximated by simple design approximations and heuristics. A multiscale framework has also been developed to combine information at the economy scale and from life cycle inventory databases with reaction pathway information (166, 167).

Systematic methods for the design of more complicated products is a relatively recent area of research, and most attention has been directed toward satisfying economic objectives. Microeconomic aspects, such as the effect of consumer behavior in the form of price-demand elasticity, have been considered while designing the products (168, 169). The grand model for product

design includes sustainability along with other objectives (170). Sustainability considerations have been included by means of LCA and life cycle sustainability assessment.

The activity of including sustainability considerations in product design is relevant to products in many areas other than chemical engineering. A road map relevant to the design of all kinds of sustainable products brought together methods such as LCA, principles such as those from the Natural Step, and business and economic considerations (171) and has encouraged the development of various approaches, particularly for the design of mechanical products. This includes heuristics for green engineering (172) and checklists for guiding product design in early stages of specific industries such as automotive (173) and packaging (174). The resulting insight supports Design for Environment (175) and has also been consolidated into principles such as the six Rs of sustainable manufacturing: reduce, reuse, recycle, recover, redesign, remanufacture (176).

Innovation is a critical bottleneck in the development of new products. This continues to be true for sustainable products as well. For the design of single molecules, reaction networks provide an array of alternatives, while for more complicated products, alternatives are often generated from heuristics or experience. In terms of the requirements for environmental sustainability, methods for sustainable product design mostly ignore their effect on ecosystem services and whether wide use of these products may exceed nature's capacity. Sustainable product design focuses on the impact of a single product, but its environmental impact is usually due to large-scale adoption of a large number of products. Thus, considering macroeconomic and behavioral impacts is particularly important in the design of sustainable products.

3.4. Dynamics and Control

Most of the work described so far ignores dynamic behavior even though technological, ecological, economic, and societal systems that are relevant to sustainable development exhibit complex dynamics. Many research efforts have focused on understanding the dynamic nature of sustainable systems, control of process and societal systems to meet sustainability goals, and control of technologies that are emerging to meet the challenges of sustainable engineering. As shown in **Figure 3**, research in this direction has been quite limited as compared to other areas of PSE.

A recent review (177) describes the large body of work and the challenges in controlling technologies that are likely to have a smaller environmental impact. These include wind and solar energy, and integration of renewable and nonrenewable resources along with energy storage options. Methods for process control of such technologies are needed, but as discussed in Section 1, sustainability requires consideration of systems larger than a single technology to reduce the chance of burden shifting.

Some metrics that consider dynamic behavior of systems were described in Section 3.1. These metrics have been used to quantify environmental sustainability along with other metrics to quantify economic and societal sustainability in dynamic systems. The dynamic behavior of integrated economic, ecological, and societal systems has been simulated as an optimal control problem to gain insight into the long-term behavior of such integrated systems. Such simulated systems can provide insight into the dynamic behavior of complex systems and their sustainability (178, 179). A theoretical framework called "sustainability on sets" is based on maintaining a dynamic system within a specified sustainable region (180).

Sustainability metrics described in Section 3.1 have been included in process control to incorporate sustainability considerations. The metrics in GREENSCOPE have been used to choose more "sustainable" operating points for systems that have multiple steady states (181). Metrics based on the sustainability vector space consisting of triple bottom line objectives (46) have also been used to guide control actions. Realizing the problem of burden shifting due to this focus
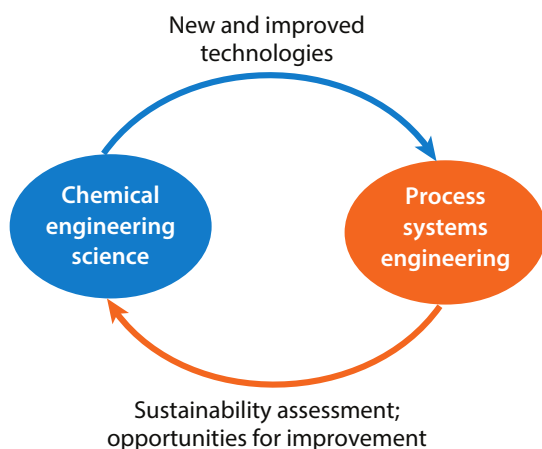
New and improved
technologies

Chemical
engineering
science

Process
systems
engineering

Sustainability assessment;
opportunities for improvement

Figure 5

Interaction between chemical engineering science and process systems engineering (PSE) for enabling
sustainability. PSE evaluates new technologies developed by chemical engineering science and suggests
modifications and innovation to reduce the chance of unintended harm.

on control of individual processes, a hierarchical control scheme is proposed in Reference 182 to
connect strategic decision makers who determine sustainable options with tactical process control
that implements the options in the process by means of control strategies such as model-predictive
control.

Dynamics and control of systems at scales of the life cycle and larger have also received some
attention. This includes the use of model predictive control for policies to address climate change
(183) and use of economic models to determine the effect of taxes on the life cycle impact of
biofuels (143).

4. PROGNOSIS

Chemical engineering has come a long way from denying its environmental impact to working
toward reducing the environmental impact due to its activities and their life cycle. In addition, mo-
tivated by the desire to contribute to sustainable development, numerous technologies are being
developed in areas such as renewable energy, process intensification, energy storage, biodegrad-
able polymers, bioproducts, waste management, etc. However, to prevent a repetition of the his-
tory of unintended harm from these and future technologies, tight integration is required between
chemical engineering science and PSE. As depicted in **Figure 5**, the new technologies developed
by chemical engineering science need to be evaluated by PSE, which in turn needs to suggest mod-
ifications and innovation to reduce the chance of unintended harm and to ensure sustainability.
Given the complex nature of interacting technological, ecological, economic, and societal systems,
the chance of unintended harm will always remain. Therefore, technologies and management sys-
tems are needed that are flexible enough to be modified and replaced as we gain experience and
knowledge about their impacts on ecological and economic systems (6). Such systems would pre-
vent societal "lock-in" into an unsustainability trap for long periods and would enable adaptation
in response to complex interactions.

As depicted in **Figure 1**, for a sustainable chemical engineering, PSE needs to expand to con-
sider larger scales all the way to the global economy and biosphere. In addition, it also needs to
account for and respect the capacity of ecosystems to support industrial and other human activi-
ties. Research and applications in PSE have certainly been moving in these directions, but some
formidable challenges lie ahead. For example, including nature's capacity in engineering decisions

can go against the traditional engineering paradigm of wanting to control and dominate nature. This paradigm has prevailed since at least the Industrial Revolution. In addition, sustainability may indicate that greater efficiency, as pursued currently in reductionist research, is not an appropriate goal. Instead, less efficient technologies may be better if the resulting waste has more use to enable a circular economy than the waste from more efficient technologies. Such changes in the practice and paradigm of chemical engineering are likely to encounter resistance that is not just cultural. For example, respecting nature's limits may require industry to convert all wastes into biological or technological nutrients to enable synergies between industrial and ecological systems. Some industries may not even remain feasible. Like chemical engineering, most other disciplines are also working toward ensuring their positive contribution to sustainable development. Examples include the use of systems thinking to enable a sustainable chemistry (184), and accounting for the role of nature in economics (185) and industrial processes (186). Eventually, convergence of engineering with ecology and economics will be needed, and a common set of fundamental insights for ensuring inherent sustainability of all activities.

Education needs to adapt to enable such advances. Advances are needed that address the relatively low ecological literacy of engineers (187). Courses on sustainable engineering are still not common in chemical engineering departments. Most process design texts and some courses do include material on sustainability, thus addressing the criticism of Cano-Ruiz & McRae (10). However, the core curriculum of chemical engineering needs to include the basic principles of sustainable engineering across all courses. Meeting all these research and education challenges involves a critical role of PSE.

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Contents

Errata

An online log of corrections to *Annual Review of Chemical and Biomolecular Engineering*
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