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PERSPECTIVE

Sustainability in the context of process engineering

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Abstract Computational process design for sustainability using various available techniques is still limited to computer-aided design featuring process optimization of energy and material flow plus minimizing greenhouse gas emission and water conservation. Sustainable process demands more, such as minimizing the impacts from other harmful emissions, discharges, waste creation, economic, and societal impacts. We have proposed an overall sustainability footprint, which in theory represents impacts of a process on all three domains of sustainability. This perspective article provides a critical analysis of attaining sustainability by minimizing this sustainability footprint using impact data as indicators. We also propose the use of the integration of the sustainability footprint in the computer-aided process design itself, rather than checking the impacts after the data have been collected on actual process options designed ahead of the analyses.

Keywords Sustainability · Process design · Process engineering · Sustainability footprint · Aggregate index

Introduction

Developing a commercial process often involves engineering concepts of process syntheses, intensification, integration, simulation, and optimization for the desired purpose of resource use and cost minimization. In a competitive marketplace, this objective is both for seeking profit and environmental stewardship. Two parallel efforts have been central to process engineering over the last two or three decades with impressive results. One of these is minimization of resource use intensity (energy, materials, clean water) that was spearheaded by heat integration and waste reduction. Later, the concept of resource use minimization was extended to mass exchange networking, and to various process and cost optimization techniques. The other effort came from the concerns for the environment and was focused on quantifying process wastes into environmental impacts, particularly of toxic materials generated, emitted, or released from processes. With lifecycle assessment (LCA) techniques taking hold among process designers, process engineering started to combine the knowledge generated by researchers who were focused on devising measures for exposures of toxic compounds to humans and the ecosystems. These two efforts have now merged into an integrated design for safer processes that are efficient and cost effective. We could call this combined approach process engineering for environmental stewardship. But the determination of environmental impacts and health effects has remained outside computer-aided process design efforts so far. The idea of sustainability, on the other hand, promoted not just the responsibility for a safer environment, but also that for promoting societal equity, both intra-generational and inter-generational. Sustainable consumption has come along as an idea in this regard.

Historically, the entire story of industrialization to date has definitely and steadily contributed to societal well-being writ large, despite creating serious environmental problems, especially of the unintended and unforeseen kind. But the current emphasis on societal equity and

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sustainable consumption is a responsibility industry is ill-equipped to handle. Proponents of sustainability have been thinking globally all along, and industrial enterprise found itself in responding to this call. A glance at any sustainability website of a large multi-national company will show that industry has taken a comparative view of sustainability. Thus the sustainability reports are always presented on a successive year over year reduction of use intensity of resources and cost, release of emissions, and discharges of wastes.

Sustainability research in process engineering can be broadly classified into two interacting categories: design of industrial process systems for sustainability, and inferring on their sustainability by measurement, the latter, a newer trend, being useful for further improvement. The first approach is prospective and the latter retrospective. When the two are integrated into one design methodology, we would have arrived at the potential of computer-aided design for sustainable processes. Efficient product and process designs have been developed over the past three decades with the help of advanced computer-aided process design tools, enabling the identification and tracking of a wide range of inputs and outputs from a process. Several such design tools have been available in the marketplace for some time. They have been used extensively for efficient designs of single-unit operations such as distillation, as well as for designing an entire process for manufacturing single or multiple products. Achieving economy in the use of material and energy resources, and cost and waste minimization has been core concerns of these prospective design efforts.

The older ideas of waste minimization, pollution prevention, and design for the environment have been focused on reducing adverse impacts on the environment and human health resulting from emissions, discharges, and handling of hazardous and nonhazardous wastes. Much work has been done in optimizing the use of materials (mainly water) and energy in computer-aided process modeling. For some time, this integration of process models with resource use minimization and cost minimization has been claimed as modeling for sustainability. LCA of impacts from resource use, although it has been in development for at least two decades, has experienced a parallel path, involving computations not imbedded in process simulation methods. Marrying these two ideas in one package would be a desirable milestone to achieve. Addition of societal impacts of exploitation of depletable natural resources to these concerns gave rise to the idea of sustainability. Life-cycle thinking, i.e., accounting for the impacts of materials, wastes, products, byproducts, and energy, is crucial to inferring overall sustainability of products and processes. Another crucial component is choosing indicators or metrics of sustainability that provide a sense of sustainability compared to a reference (thus comparative sustainability). The overall goal is to achieve environmental, economic, and social benefits, in keeping with the definition of sustainability. In this paper, we discuss the two major research directions, mentioned above in sustainable process engineering. We also show that an overall sustainability footprint can be devised and sustainability concerns be directed to minimizing it.

Sustainable process design

Traditional process design translates chemical synthesis to a chemical process (Diwekar 2003) containing a network of process units and connections, each of which serves a function in delivering the product of interest. Process systems engineering (PSE) deals with the understanding and development of systematic procedures for the design and operation of batch and continuous process systems at multiple scales (Grossmann and Westerberg 2000). Within PSE, various methods can be used to study the sustainability of process systems. The methods broadly encompass process integration (dealing with the material and energy flows within a process system) and process intensification (dealing with reduction of the number or size of process equipment within a process system). Both of these methods ultimately lead to the economic and environmental benefit of the process system as a whole.

A newer trend in sustainable process design is inspired by the desire to reduce resource and energy use intensity as well as environmental impact by making use of environmentally friendly, renewable raw materials, and fewer solvents. This approach may involve newer chemistries, for instance, a biological route in preference to a chemical one.

The advent of advanced computing tools, such as Aspen Plus® (2014) which has detail thermodynamic properties, Aspen HYSYS® (2014) for a quick design with minimal information that is available, gPROMS® (2014) mainly for dynamic process simulation, PRO/II® (2014), etc., has immensely helped the development and analysis of chemical process systems. The initiatives by the CAPE-OPEN Laboratories Network (Co-LaN 2014) have helped in promoting the use and development of CAPE-OPEN standards used in the standardization of process modeling tools. These design tools, however, have rarely looked at environmental impacts. This therefore is a need in computer-aided sustainable PSE.

Process integration

In chemical engineering, process integration took the first step toward sustainability through heat and mass integration. Mass exchange networks (MENs) naturally followed the forerunner, heat exchange networks (HENs), because the two concepts are tied together by the constitutive equations of continuity and motion, which processes must obey.

Heat integration

Processes require both heating and cooling at various stages in their flowsheets and HENs help conserve heat energy, needed in managing reactions and effecting species separations. Early work by Hohmann (1971) showed how energy economy can be achieved in a process by optimally transferring heat from hot streams to cold streams. Optimization of HENs for energy use minimization provides answers to questions such as which hot and cold streams can be matched and what optimal heat load is to be added or removed from them, and in what sequence. This is achieved by Pinch Analysis, using either graphical or algebraic methods. The graphical method introduced by Linnhoff and Flower (1978) constructs a pinch diagram to find the maximum heat exchange among process systems through minimum usage of utilities. A thermal exchange pinch point is identified on the hot and cold composite curves where the two streams touch each other. No heat must pass through the pinch, no cooling utilities should be used above the pinch, and no heating utilities below the pinch. HEN Optimization technique was mainly developed by Papoulias and Grossmann (1983). It was further developed with retrofit design by Asante and Zhu (1996), Klemeš and Bulatov through integration of waste and renewable energy (Perry et al. 2008), Kravanja (Yee et al. 1990), and many others. Reviews were provided by Gundersen and Naess (1988) on heat integration, and by Linnhoff (1993) on pinch analysis. A critical review of HEN synthesis was provided by Furman and Sahinidis (2002).

There are several commercial tools available for heat and mass integration (Bulatov 2013a, b). For example, Aspen Energy Analyzer is available with ASPEN Hysys® (2014) and Aspen Plus® (2014). It allows optimal design of HEN along with Pinch Analysis. Process Integration Limited has various design tools for specific application of heat integration: CDU-int (2014) is for heat integration in crude oil distillation system, DIST-int (2014) is for integrated distillation systems, HEAT-int (2014) is for individual process, SITE-int (2014) for site utility systems in process industries, etc., HEXTRAN (2014) is another efficient tool for different types of heat exchanger and network design. It has features to evaluate complex systems and it performs retrofit design. SPRINT (2014) developed by University of Manchester can be used to design energy systems for individual processes. It allows choice of utilities to perform energy targeting in the process. STAR (2014) is another software developed by University of Manchester. It is used for the design of utility and cogeneration systems. SuperTarget is heat integration software introduced by KBC (2014). It takes data from different commercial tools through interfaces and performs HEN design. Another software, WORK (2014) can be used for heat integration of complex refrigeration systems.

Mass integration

In PSE, the goal is to maximize product yield by minimizing resource use and environmental impacts, while also minimizing energy use. Introduced by El-Halwagi and Manousiouthakis (1989), and greatly expanded by El-Halwagi (2011), mass integration by way of MEN uses the knowledge of the flow of mass within the process in identifying performance targets and optimizing the generation and routing of species in the process. Three types of mass integration goals are minimum waste discharge, minimum purchase of fresh raw material, and maximum product yield—thus a multi-objective optimization problem. To achieve mass integration, the process may have to undergo modifications through stream segregation, mixing, recycling, interception, or has to incorporate changes in design and operating condition of units, substitute materials, or technology changes that use alternate chemical pathways. Process changes for mass integration can be categorized as no- or low-cost changes, moderate cost modifications or entirely new technologies (El-Halwagi 1999). Mass exchange units in MEN identify mass separating agents (MSA), such as a solvent or an adsorbent that selectively removes targeted species, such as a product or a pollutant. In the optimization problem, the exchange units and MSAs are chosen, they are paired with rich streams, and the optimum flows of MSAs found. The construction of a pinch point in a mass exchange pinch diagram, where rich and MSA composite streams touch, facilitates the realization that no mass should pass through the pinch, no external MSAs should be used above the pinch and excess capacity of process MSAs should not be removed below the pinch. A review of water networks in refineries and process plants is given by Bagajewicz (2000). Water integration with recycling in industries is shown by Alnouri et al. (2014). Other important review on water minimization was given by Foo (2009), Jeżowski (2010) and on general mass integration by El-Halwagi (1998), Dunn and El-Halwagi (2003).

Unlike tools for heat integration, there are very few commercial tools available for mass integration. Most of the tools are limited to water and hydrogen networks. H2-int (2014) developed by Process Integration Limited and HyNDT™ (2014) developed by Technip are commercially used for hydrogen integration. WaterTarget^{TM} (2014) is a commercial tool developed by KBC for simultaneous design of water reuse, regeneration, and treatment. Among the academic tools available, Optimal-Water© (2014) is a Microsoft Windows-based program developed by PROSPECT, Universiti Teknologi Malaysia which computes the minimum water and energy requirements, WATER (2014) is a software package developed at the University of Manchester for designing water systems in process industries, and Water Design (2014) is a Windows-based tool developed at Virginia Polytechnic Institute and State University which generates freshwater use/wastewater targets, identify bottlenecks for water reuse, and finding new reuse opportunities. MEN provided by El-Halwagi (El-Halwagi 1997) aids in design of waste recovery networks using algebraic and optimization-based techniques. This tool is not restricted to water or hydrogen and can be used for minimizing the cost of MSA. It requires user input of supply and target composition, maximum MSA flowrate, solute distribution, cost, and some other parameters for lean streams, and supply and target compositions and flowrates for rich streams. RCNet (Ng et al. 2014) is a spreadsheet tool based on Microsoft Excel for the synthesis of resource conversation networks (RCN) for the efficient use of material resources (e.g., water, utility gases, solvents, etc.,) in industrial plants. This tool is the first of its kind to handle water minimization, hydrogen recovery, and property integration, and solve these problems independently in a single interface.

Process intensification

Some existing processes can be made safer, more efficient through the use of advanced process equipment. The concept of process intensification was pioneered by Colin Ramshaw and his co-workers more than thirty years ago when they developed a rotating packed bed for reactive distillation (Ramshaw and Arkley 1983). Since then, process intensification has evolved to be an integral part of retrofit designs, and resulted in enhanced economic and environmental benefits, and has been identified as a key technology for the realization of sustainability goals (Tsoka et al. 2004). Research in process intensification encompasses process intensifying equipment (spinning disk reactors (Mukherjee et al. 2001), multifunctional heat exchangers (Ferrouillat et al. 2006), microreaction, structured catalysts, and process intensifying methods such as reactive separations, hybrid separations, and process synthesis (Linke et al. 2008). Primarily, the mechanisms involved in process intensification result in enhanced heat and mass transfer. Intensified heat transfer occurs through the development and use of active (use of external power) or passive techniques (Reay et al. 2013). Examples of passive techniques include treated or rough surfaces, displaced enhancement devices, swirl flow devices, coiled tubes, surface catalysis, etc., and active techniques include mechanical aids, surface vibrations, fluid vibration, electrostatic fields, rotation, induced flow instabilities, etc. Mechanisms involved in intensified mass transfer are rotation, vibration, mixing, etc. Some of the methods for heat transfer enhancement can also be used for intensified mass transfer, e.g., rotation (in a cyclone or a rotor), vibration, and mixing. Other than these, electrically enhanced processes, microfluidics, and pressure driven processes have also gained importance in process intensification. Simultaneous separation and product design has been reported by Eden et al. (2004) and later on process synthesis as a method for process intensification by Lutze et al. (2010). Recently, membrane engineering for process intensification has been reviewed by Drioli et al. (2011). A key aspect of research in process intensification involves process control, and has been reviewed by Nikačević et al. (2012).

Recently, process integration and intensification have gained attention as way to achieve sustainable process development. A review on process integration and intensification is given by Klemeš and Varbanov (2013), Varbanov and Seferlis (2014). García et al. (2014) showed application of process intensification in a biorefinery using ultrasound technology. Process integration for cogeneration and integrated energy systems is shown by Kamrava et al. (2014) and Benjamin et al. (2014), respectively.

Designing sustainable processes by pollution prevention

Because sustainability is comparative and technologies change with time along with environmental regulations and stricter societal demands for protections from chemical exposures, no process can be developed that can be called sustainable forever. Still, some general guidance can be used, such as avoiding toxic materials, using non-fossil energy sources as practicable, practicing recycle/reuse, producing byproducts for beneficial use, etc. This approach is akin to what Intel Corporation called beyond compliance. The essential idea is pollution prevention that includes avoiding unintended consequences. Specific guidance for specific industry sectors can also be suggested. For instance, sustainability of solar photovoltaics will depend on materials use efficiency, secure access to rare earth materials, minimizing cost and waste generation in manufacturing solar cells, minimizing water and energy use in manufacturing and in array washing, and unintended consequences on wildlife such as protected bird species. For wind power, it would be paying attention to material use and cost of turbine and support structure manufacture, secure access to rare earth materials, and protection of birds from rotating turbines. For biomass for fuels, sustainability will depend on water use, greenhouse gases (GHG) emission from tilled soil, cost, and adverse impact on energy–food nexus. For coal to be a viable fuel for the future, its environmental impact must be reduced. Its carbon footprint can also be reduced by cost-effective capture and sequestration of CO_2. A step forward toward sustainable mining would occur if water management can be significantly improved, and waste management is vastly improved by recovery and recycle. Plastics manufacturing can improve its sustainability performance by complete recovery and reuse of organic solvents in manufacturing, and by designs that enhance post-consumer recycle/reuse. In the design phase of any process in any manufacturing sector, LCA thinking should always be employed for reducing adverse environmental and health impacts due to upstream and downstream factors of a process being designed.

Developing design methodologies that include sustainability analysis

Computer-aided process design is limited to using integration techniques discussed above that treat energy and some resource use concerns. Recently, concerns about global warming, as expressed in emission of GHG, are also included in some PSE designs. Societal impacts are not explicitly addressed, as it is difficult to know what specific societal indicators for which a process should be accountable for. At the scale of a manufacturing company, inclusion of societal indicators is easier rather than at the process level. So long as societal impacts due to a process are expressible in human and ecological health impact terms, these impacts should be but not yet incorporated in the computer-aided design packages. Life-cycle impact assessment program such as tool for the reduction and assessment of chemical and other environmental impacts (TRACI) (Bare 2014) does include some health impact estimates, but the models used for these estimates could stand upgrades from the use of newer computational toxicology models that cover predictions of additional health and ecological impacts that TRACI does not yet include. Moreover, material and energy intensity, and GHG emission, from a sustainability point of view, need to be from a cradle-to-grave (C2G) LCA viewpoint. But a comprehensive LCA accounting methodology of this type, though appreciated in principle, is not yet available in the form of a publicly available computer software. In practice, the data needed for the task are not readily and publicly available and generally they suffer from data interoperability and standard definitions. And they are expensive to collect. Thus, current ready-to-use designs methodologies are largely gate-to-gate (G2G), which nonetheless have their utility in informing the process designers of G2G impacts of competing processes for the same product or products. In cases involving similar inputs and outputs, the G2G methods approximate C2G, because the inputs and outputs nearly cancel out. C2G LCA is exceedingly complex and difficult to reduce to a computer-based formalism. Thus the practitioners have to analyze for sustainability with life-cycle data as a feedback complement to computer-aided process design using measured values of indicators that represent the optimized process.

Indicators for sustainability evaluation

The sustainability of a designed process is measured by a set of indicators that reflects the impacts of the process on the environment, society, and the economy. A particular process can be incrementally made more sustainable by improving one or several indicator values, all other impacts remaining roughly the same. Typically in choosing among several alternatives, however, an overall comparative analysis must be made to claim relative sustainability of a process or a product. Not a set of identical indicators can be applied to all manufacturing systems, but for chemical processes the concerns are roughly similar. We propose that core indicators for chemical processes should embrace the following nine concerns: energy use, material use, water use, wastes generated, hazardous compounds emitted, land use, cost, process safety, and harmful emissions from products. The actual embodiment of these concerns can be in the form of a collection of core indicators for these concerns augmented by supplemental indicators from each concern, as needed. Generally, however, fewer indicators are preferred, as they will likely be adopted by industry. Such suggested indicator sets, that address some of the nine core concerns mentioned above, are available from professional societies and specific chemical companies. Sikdar et al. (2012) illustrate some of these indicator sets, most containing less than 10 indicators in total, and their use. On the other end of the scale, a methodology called GREENSCOPE created by Ruiz-Mercado et al. (2012) for process evaluation that calculates about 140 indicators that belong to categories of environment (GWP, acidification potential, eutrophication potential, etc.), material efficiency, energy efficiency, and economics (profit, net present value or NPV, return on investment or ROI, etc.). After the indicator data have been collected, typically the decision making is made by plotting the indicator values on a spider diagram (Shonnard et al. 2003), and looking up for the most sustainable alternative. This visual method is fraught with difficulties when the number of indicators is large or the process alternatives too many.

Decision making with sustainability indicators

The spider diagram approach has its utility in identifying which particular indicator needs to be improved by process modification of an existing process or in a comparative analysis of several alternative processes. This comparative analysis can be greatly simplified, however, if the indicators can be rationally aggregated into a single index. Additionally, one has to be warned against using multiple indicators derived from the same concern. Such uses can introduce bias in the analysis. Also, one needs to be able to determine the relative contribution of the indicators to sustainability to enable one to pay particular attention to their role in improving process design or redesign, Sikdar et al. (2012) have shown that aggregate indicators based on the concept of Euclidean distance or the geometric mean of the ratios of indicators of a system to those of a reference system provide two alternate ways of indicator aggregation. We called the aggregated index as the sustainability footprint of engineered processes. Mukherjee et al. (2013) demonstrated that the set of indicator values together with the sustainability footprint can be subjected to multivariate statistical analyses using partial least squares variable importance in projection (PLS-VIP) to reliably choose the most sustainable process alternative and also provide the set of indicators that are minimally needed to make a decision on sustainability, thus addressing the issue of indicator sufficiency and redundancy. Recently, Sengupta et al. (2015) showed the application of sustainability footprint and multivariate analysis for decision making regarding sustainability in various engineering systems. It needs to be emphasized here that sustainability analysis as discussed in this section is retrospective. The indicator data have to be available on existing process alternatives for such analyses. This approach is useful in process redesign.

Integrated computer-aided process design

The classical computer-aided process design can subsume the environmental, societal, and economic concerns in an integrated design methodology. The inclusion of mass exchange networking and GHG emission minimization in the way of multi-objective optimization has been a good start in this direction (Diwekar 2003; Guillén-Gosálbez 2011). This would then effectively make process design prospective by combining the two trends toward sustainable process design we have discussed before. The challenge in this endeavor is that the process being designed does not yet exist and indicator data, especially on health impacts, are not available. One way that can be suggested would be put an impact assessment module inside the process design methodology, and for processes that do not yet exit, estimate the identified impacts from archival data. The resulting multi-objective optimization would now be an expanded task of optimization among process efficiency, cost, and all relevant sustainability indicators that have been chosen. The vastly increased dimension of the objectives can be reduced to simply using the sustainability footprint as a surrogate. We suggest this approach not because it is simple but it would hopefully be simpler by achieving the task of combining computer-aided process design with the off-line sustainability assessment.

Conclusions

Great strides have been made in computer-aided PSE in the last several decades, and several competent products are available in the marketplace to assist us in the endeavor. Even before the idea of sustainability penetrated the chemical engineering discipline, heat, and mass integration started to make some progress toward energy and material resource optimization in a designed process. These are fundamental to the idea of sustainability, which stipulates resource use minimization as an important component of sustainability. The other components are economic viability, environmental stewardship including safeguarding human health, and societal good. There are some opportunities for PSE for developing processes that can be evaluated as potentially more sustainable compared to an extant process. In other words, computer-aided process engineering can provide a prospective design methodology for sustainable processes. Some researchers have taken the approach of pollution prevention or green chemistry in designing a process from scratch, from the ground up, so to speak, using chemicals and materials that are benign to begin with and by choosing chemical syntheses that produce little or no byproducts. Having a hopeful chemical synthesis is, however, not the same as a sustainable process. There would have to be a way to verify claims of sustainability that can be achieved in the relative absence of data. Advanced PSE can fill this important innovation gap.

A process has an upstream side with materials, energy, and labor input over which a manufacturer has limited control. The downstream side consists of products getting in the hands of the consumers, wastes getting dispersed, or being treated or shipped to landfills. LCA requires that the environmental, societal, and economic impacts of these upstream and downstream material and energy flows be known. The process owner has almost complete control over the process, and he can make the process as clean as he wants, provided he can afford it, but for sustainability the dilemma is that he must know ways of estimating these upstream and downstream impacts. In other words, he is in need of a PSE package that can assist him with the LCA.

There are LCA packages that can assist him alright but these are mostly off-line calculations. The integration of LCA into the PSE package is an important need for the near future. Another need is for the PSE packages to allow making sustainability decisions. We have provided in this manuscript some ideas of what needs to happen for PSE to transition from the current state of material, energy, and cost optimization to sustainability decisions.

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