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Sustainable Process Systems Engineering – You're Doing It Wrong!

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ABSTRACT

Most studies in process systems engineering are applying incomplete methods when incorporating sustainability. Including sustainability is a laudable goal, and practitioners are encouraged to develop systems that promote economic, environmental, and social aspects. Ten methods that are often overlooked in performing sustainable process systems engineering are listed in this effort and discussed in detail. Practitioners are encouraged to create designs that are inherently safer, to be more complete in their identification of process chemicals used and released, to be complete in their definitions of supply chains, and to apply additional environmental impact categories. Other methods point to items that are factors in process systems engineering such as disruptive recycling, robust superstructures for optimizations, and employing complete sets of objectives. Finally, users should be aware that sustainability tools are available, which might have been outside of their awareness.

Keywords: Optimization, Process Design, Supply Chain, Life Cycle Analysis, Environment, Sustainability

INTRODUCTION AND BACKGROUND

Practitioners of process systems engineering stand at the cusp of chemical process design / analysis and life cycle assessment. For those interested in sustainability the methods available to users are growing in popularity but perhaps remain still largely unknown.

In an effort to promote sustainability, studies that developed into the modern methods of life cycle assessment (LCA) were first reported in the 1960s [1]. These studies considered cumulative energy use and comparisons of different beverage containers to quantify the use of natural resources and releases to the environment. Today, rules are being set to formally compare products within categories [2], and LCA studies can model regions [3] and the whole economy [4].

Unlike the above evaluations of supply chain (i.e., cradle-to-grave) sustainability, efforts to optimize chemical processes have smaller single-system domains. The potential addition of new chemicals or technologies into a process makes them open ended, and demonstrated methods for the conceptual design of processes are available [5]. A subset of the open-ended problems can be optimized, and this is where various process system engineering methods realize their power.

These fields cross pollinate as described in a review of design methods for the environment by Cano-Ruiz and McRae [6]. Alternative generation for designs is combined with optimization methods. One can consider the sustainability of processes within a system by continually expanding the system boundaries to the enterprise, life cycle, economy, and ecosystem [7]. Most studies which make an attempt towards sustainability are incomplete, and so a listing of commonly overlooked methods is offered here.

TEN UNDERVALUED METHODS OF SUSTAINABLE PROCESS SYSTEMS ENGINEERING

Awareness of methods to improve sustainable process and system design are available as listed in Table 1. Following the table, a series of descriptions will be provided to describe each item in more detail.

Table 1: Ten methods for sustainable process systems engineering that are undervalued.

Number	Name
1	Use Inherently Safer Designs
2	Incorporate Inputs / Outputs of Complete Supply Chains
3	Account for All Chemicals and Releases
4	Define Final Fate / Destination for Every Chemical
5	Include All Emissions, Discharges, and Solid Wastes
6	Apply Additional Impact Categories
7	Recognize the Disruptive Nature of Recycling to Design / Optimization
8	Create a Robust Superstructure of Alternatives
9	Use Complete Sets of Objectives
10	Realize Sustainability Tools are Available

Use Inherently Safer Designs

Inherently safer designs avoid circumstances that could cause accidents as well as chemicals that are unnecessarily toxic. This is one of the original principles of green chemistry, which are listed along with engineering principles in one reference [8]. While not repeated here, the intent is to include all of these principles in this listing of methods for process systems engineers to consider. Only designs that advance these principles will be aligned with sustainability.

Incorporate Inputs / Outputs of Complete Supply Chains

Designing chemical processes is an open-ended problem with the potential to introduce various chemicals to be part of a product formulation, reacted, or to ease processing. Each chemical introduced requires its own supply chain of processes to manufacture and transport the used chemical. This complete inventory of reactants, solvents, catalysts, processing aids, and cleaning agents is not simple to assemble [9], but the reaction products may be a much longer and less well-known list. Each of these byproducts should be considered for where it ends up and the output system of processes required to handle non-products. Some of these non-product processes may involve flaring, wastewater treatment, hazardous waste treatment, or recycling, each with its own supply chain and releases to the environment. Many of these processes are never seen in studies that show process system diagrams. Therefore, in many cases of process design and analysis, it can generally be concluded that little attention is paid to the fact that every input / output to / from a system requires an upstream / downstream supply chain.

Account for All Chemicals and Releases

The reactions most process systems engineering studies and life cycle inventory databases consider are overly simplified. As an example, acetic acid production can be modeled according to the stoichiometry of carbon monoxide and methanol reacting to form acetic acid. The actual components found in a real process are often much higher [10]. Beyond the process inputs, chemicals might be introduced to a process for a number of reasons: absorption, boiler feedwater circulation, catalysis, cleaning, cooling tower circulation, input water treatment, wastewater treatment, etc. Some examples of these are presented in the context of early-stage process development [11]. All of these inputs might be released to the environment. In addition, boilers, cooling towers, and fugitive emissions can dramatically increase the number of chemicals released to the environment.

Define Final Fate / Destination for Every Chemical

When considered holistically, one can envision that every chemical must eventually be reacted, recycled, released, or treated. Certainly, some chemicals go into products, but holistically they will have to realize one of these fates. The challenge for the practitioner of process systems engineering is to logically identify the chemicals present and then track their fates. First, one can apply a version of the methodology described by Douglas [12] where each reactor effluent component is given a destination code. Products and by-products exit as product streams, but impurities of these products will likely be in other streams. In addition, consider that there will be other impurities in the product streams. Unused inputs will mostly be recycled, where possible, but input impurities and unrecycled quantities will exit in various streams. Some streams may have a high enough energy content to legitimately be used as fuel. The other streams will exit as process wastes, where their phase will dictate their form and whether they are vented, process liquid wastes, or solid wastes. Where captured, each of these can be treated with absorption, flaring, land disposal, thermal oxidation, wastewater treatment, etc., and each of these processes has its own resource use and releases to the environment [13]. In addition to exiting in the paths described above, the uncaptured chemicals (some of which will be valuable products, reactants, etc.) may be released or exit as fugitive emissions.

Include All Emissions, Discharges, and Solid Wastes

In designing and analyzing processes, the releases to the environment include air emissions, liquid discharges, and solid waste. Air emissions are the best represented and analyzed of the releases. The most common of the reported air emissions are greenhouse gases

(GHGs), which are easily determined through calculations of energy type and amount used.

One can speculate that the search for data that is relevant to environmental impact categories suffers from the "streetlight effect". This effect is told as a story of someone looking for their keys under a streetlight, and a passerby who stopped to help look for them finally asks where the keys were dropped. The answer is two blocks away, but the light is better here, with the analogy for emission data being the easy-to-see GHG data. Other forms of bias, like availability, can play a role as well, as that bias selects easily recalled items as being important. In general, analyses would benefit from not prescribing what important emissions, discharges, and solid waste flows are in advance of evaluations.

To improve process models that have been ignoring storage, transfer, vent, and fugitive emissions as well as liquid discharges and solid wastes, a number of methods are reviewed in the literature [10]. In addition, specific methods for estimating emissions for unit operations such as boilers, loaders / forklifts, and cooling towers are available [11].

Apply Additional Impact Categories

The number of human health and environmental impact categories included in most studies are very limited. Global warming potential is often incorporated, but many other categories are dismissed through omission. I.e., no one has made a conscious decision to give a zero weighting to other categories; they have simply been omitted. Even in examples where more categories are used, the number is still relatively small [14]. A more extensive taxonomy of environmental impacts is available consisting of many tables of detailed midpoint effects (e.g., global warming potential (GWP) is a midpoint effect determined from emissions), endpoint effects (e.g., skin cancer, reduced lung function), and damage groupings (e.g., disability adjusted life years) [15]. Seldom, if ever, will a study use all of the available impact categories, but a review of those that are available can inform a more complete analysis, i.e., one in which more categories are included, or the text better describes the intent and caveats of the system analysis.

Recognize the Disruptive Nature of Recycling to Design / Optimization

In chemical engineering process design, an early lesson is the effect a recycle loop can have on a design. Whereas in a straight-line process, or single-pass process, the highest yield is the best use of raw materials, when a recycle loop is added the optimum conversion can move towards the highest selectivity for use of raw materials. Recycle loops can return raw materials to the reactor system to react them more efficiently at higher selectivity. The optimum is often balanced by larger equipment and recycle streams that can increase energy use and costs.

The advantages of recycling along a supply chain are somewhat different. For post-consumer use materials, a meta-analysis using 366 datasets for 14 materials was performed, and the mean GWPs for secondary production were better than the mean GWPs for primary production (i.e., with virgin materials) [16]. However, experience has shown that the quality of recycled materials is not equivalent to virgin for many reasons (e.g., for PET plastic bales other materials are present, and for PET items other materials are part of their composition) [17]. Thus, the secondary production process is different from the primary one. This represents a radical divergence from internal recycle loops in chemical processes, where higher selectivity accomplished with more recycling leads to less impurities.

For both process systems and supply chain systems, recycling must be evaluated. A combined analysis was done for producing waste-recycled feeds using styrene "tar" from the bottoms of a styrene-refining column [18]. There is no generalization to make regarding the desirability of recycling such streams, as the system depends both on the technology and the materials recycled and produced. A practitioner of process systems engineering would do well to design and analyze each system.

Create a Robust Superstructure of Alternatives

In process systems engineering a common problem studied is the superstructure-based reactor synthesis. An early paper on the subject used a recycle reactor with heat exchange as the basis [19]. More recently, superstructure methods were applied to complex sets of reactions modeled with uncertain inputs and limiting reagents [20]. The process synthesis problem is aimed at achieving a conceptual design that identifies the operations to do. A similar larger-scale problem is challenging at the process level when new chemicals can be introduced into a process [5]. In each case the idea is to have a robust superstructure of equipment and interconnections that is flexible enough to capture designs when applying optimization. Further, at a larger supply chain scale the analysis of designs is challenging when new chemicals are introduced, as up- and down-stream processes and their resource use and environmental releases will be affected.

Use Complete Sets of Objectives

In the real world, decisions are not simple because there is seldom a real-world decision that only has one objective. Our models of processes and systems can diverge strongly from this generalization, as assumptions are made to only consider a single dimension. In process design, one might optimize economics, flexibility, controllability, safety, and environmental impacts. The GREENSCOPE tool of Ruiz-Mercado et al. has approximately 140 indicators in the four E's of Environment, Economics, Energy, and mass Efficiency, thus providing many possible objectives to optimize chemical processes [21].

There are various ways of handling multiple objectives. One method is to rearrange an objective as a constraint on acceptable solutions. Solving over a range of different values for the constraint will create a series of solutions. Another method to address multiple objectives is to normalize each objective (i.e., dividing by a maximum possible value is one normalization), weighting the multiple objectives with respect to each other, and finally adding the objectives together on a single scale. A method for applying these steps using marginal rates of substitution and total utility is described by Smith and Ruiz-Mercado [22]. Others may approach the multiple objectives through the simultaneous development of many Pareto solutions, although dimensionality issues require a method for spacing solutions among the various objectives [23].

Realize Sustainability Tools are Available

In designing or analyzing process systems it may be that people are unaware of tools that are available. Examples of tools one can use to further sustainability include GREENSCOPE [21], release estimation [11], and LCA [4] tools. In addition, solvent replacement and toxicity prediction methods are available from the U.S. EPA's Office of Research and Development (ORD). The Program for Assisting the Replacement of Industrial Solvents (PARIS) allows one to quickly find solvent replacements (either individual solvents or mixtures) that are similar in physical and chemical properties to the original. The program also provides a calculation of potential environmental impacts in eight categories, from global warming potential, ozone depletion potential, acidification potential, and smog potential, to four categories of potential toxicity [24]. Additional toxicities and many other physical properties can be estimated with the Toxicity Estimation Software Tool (TEST), also available from EPA's ORD [25].

DISCUSSION

Practitioners of process systems engineering are encouraged to employ the above list to improve their chemical processes and associated supply chains. To summarize the above, one should first create designs that are inherently safer, including other principles of green chemistry and engineering. Sustainable research and development breakthroughs advanced through sustainable chemistry and engineering improve system performance while reducing environmental burdens and economic and social costs. In the absence of breakthroughs, one can only optimize systems to make them more sustainable.

Practitioners should also be as complete as possible in their identification of process chemicals used and released, be more complete in their definitions of supply chain processes, resources used, and releases, and apply additional environmental impact categories as appropriate.

Users are likely already familiar with recycling, superstructure optimizations, and creating sets of objectives. This effort simply advises to employ these in a manner that positively disrupts systems, defines the widest possible variety of system structures, and includes complete sets of objectives. This setting of objectives, as choices of objectives, constraints, and boundaries of what is included and excluded, is critically important in defining the scope of studies.

Finally, users should be aware that sustainability tools are available, which might have been outside of their awareness. In the end practitioners of process systems engineering will likely still limit their studies with incomplete methods for sustainability, but perhaps the listing here can be used as a checklist to address what could be considered and help refine some future work.

DISCLAIMER

The views expressed in this article are those of the author and do not necessarily represent the policies or views of the U.S. Environmental Protection Agency.

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