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Review

Methodology for Assessment and Optimization of Industrial Eco-Systems

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Abstract: There is an emerging trend in evaluating industrial activities using principles of industrial ecology because of the emphasis on sustainability initiatives by major process industries. Attention has also been targeted at developing planned industrial ecosystems (IEs) across the globe. We point out the current state-of-the art in this exciting discipline and subsequently identify the challenges that have not been encountered by the scientific community yet. Ecological Input Output Analysis (EIOA) may be considered as an "all-inclusive model" for the assessment of an IE because of its ability to capture the economic, environmental, and societal behavior of an IE. It could also be utilized to illustrate the detailed inter-relationships among the entities of an IE. Optimization of a fully integrated IE using conventional multi-objective optimization techniques would be too complex. For such multi-objective optimization problems, Hierarchical-Pareto optimization discussed in the literature has shown promise, but there is a need to establish a methodology to assess and/or improve the robustness of an IE using such techniques.

Keywords: industrial eco-system; robust optimization; hierarchical optimization; emergy; ecological input output analysis; sustainability indicators

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1. Introduction

The chemical industries across the globe have started realizing the need for sustainable development, which not only addresses productivity issues, but also encompasses environmental and social responsibility. There is also an enormous drive behind the use or promotion of the term "sustainability". A widely accepted definition of sustainability or sustainable development is that given by the World Commission on Environment and Development: "forms of progress that meet the needs of the present without compromising the ability of future generations to meet their needs". Another interpretation of sustainability implies that the ecological base available for current economic activity should also be available to future generations for their needs [1].

Closely related to sustainable development is so-called "Ecology," which captures the interactions between organisms and the environment in which they occur. We can study ecology at the level of the individual, the population, the community, and the ecosystem. The study of ecosystems mainly includes establishing the relationship of the living, or biotic, components to the non-living, or abiotic, components through physicochemical processes, such as energy transformations and bio-, geo- and chemical cycles. All ecological processes are driven by independent primary energy sources, such as solar, tidal and geothermal. An ecosystem may be viewed as a network of ecological processes that transforms energy from the primary sources to produce ecological goods such as wood, coal, and water, and services such as carbon sequestration, rain, and wind [2].

Allenby and Richards [3] have illustrated an analogy between the biological and industrial ecosystems (IE). The various actors in industrial systems such, as raw material suppliers, component manufacturers, consumers, waste handlers, or recyclers are analogous to biological organisms. As defined by Nicholas Gertler [4], an industrial ecosystem is a community, or network, of companies and other organizations in a region that choose to interact by exchanging and making use of by-products and/or energy in a way that provides one or more of the following benefits over traditional or non-linked operations:

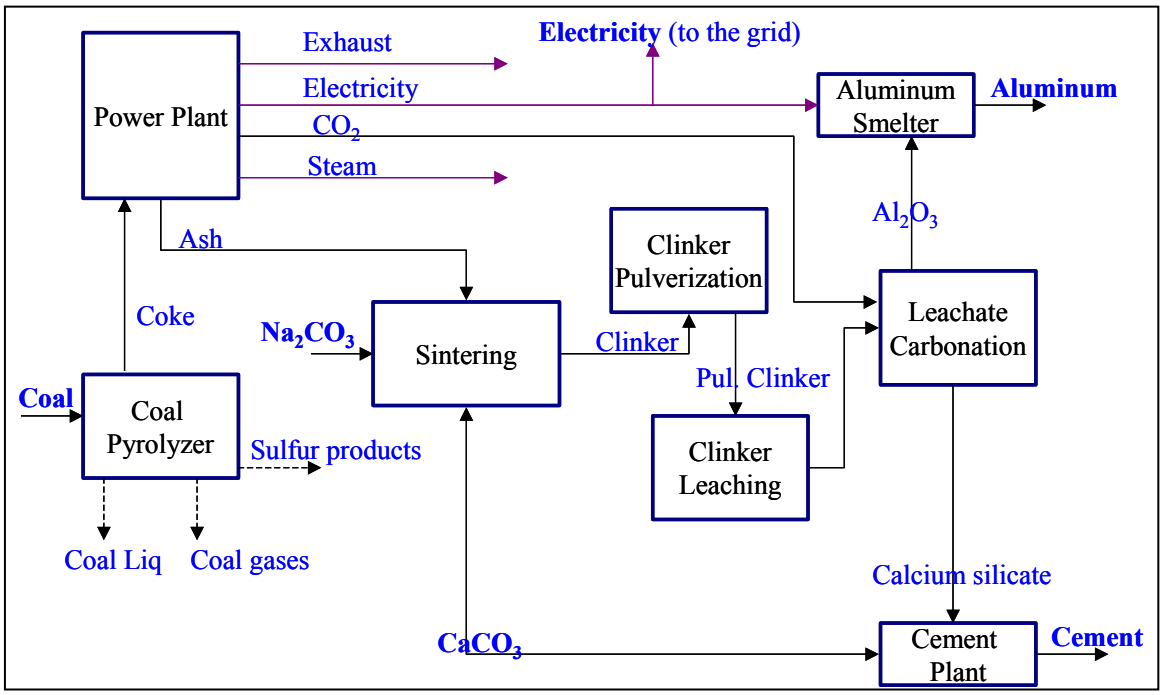
(i) Increased systemic energy efficiency leading to reduced systemic energy use.
(ii) Increase in the amount and types of process outputs that have market value.

Thus, in an integrated industrial complex there is an exchange of materials and/or energy between different industrial sectors where the output of one industry (main product or even the "waste") becomes the 'feedstock' of another. For example, excess steam or exhaust from a thermal power plant can be used as a heat source for a nearby chemical industry or in a coal-fired thermal power plant; fly-ash may be used to make products used in buildings and construction, such as aluminum and cement, as shown in Figure 1.

Thus, the current, increasing focus on "Industrial Symbiosis" warrants a new business or operating model for industry. It also demands modifications to, or the establishment of, new public policies, technologies and managerial systems which would facilitate production in a more cooperative manner. Sustaining industrial ecology draws parallels and grows along with the concept/concerns of environmental ecology. Implementing industrial ecology may involve closed loop processing, reusing and recycling, design for environment and waste exchange. Technologies and processes that maximize economic and environmental efficiency are popularly referred to as eco-efficient. Eco-efficiency refers to

a process that seeks to maximize the effectiveness of business processes while minimizing their impacts on the environment [5]. Although industrial symbiosis is not necessarily an outcome of technology advancement or breakthrough, the combined use of existing technology solutions can be an innovation itself.

Figure 1. Example showing part of an Industrial Ecosystem.



In this paper we critically review the published literature on industrial ecosystems with the aim of distilling out the methodology for assessment and optimization of industrial eco-systems. First, we briefly review the efforts undertaken by the process system engineering community, and then we discuss a few important examples of industrial eco-systems to evolve a common understanding of what its constituents are. In the later sections we discuss the basis for the sustainability assessment of industrial eco-systems, conventional optimization approaches adopted for the problems closer to IE such as green process networks, and issues/challenges with the conventional sustainability assessment and optimization approach. In the last part, we present a more realistic approach for sustainability assessment and optimization, based on available open literature. In addition, we will include a final part, comprising a proposal for a framework to assess the robustness of IE.

2. Process System Engineering (PSE) in Chemical Process Industries

2.1. Developing Optimization Techniques

Traditionally, the Process Systems Engineering (PSE) community develops process optimization models at a plant level to assist plant operations or design a new plant [6]. Various tasks involved in the process optimization exercise can be divided into two broad areas (or sub disciplines), which are further integrated by the PSE community. The first area includes formulating mathematical models based on the chemical engineering principles to establish a relationship between the system performance parameters,

such as product quality, throughput, cycle time, *etc*., and the factors affecting these parameters, such as the process variables. Typically, these models are deterministic in nature, represented by objective functions, while ensuring that the models operate within established limits enforced by constraints. But in a real-life situation, as a result of uncertainties involved either in model parameters, process conditions or external factors, the models could be stochastic in nature.

The other area of process optimization deals with the selection of a proper optimization algorithm to find the solution using the theory of optimization. Biegler and Grossmann [7] have reviewed the solution methods of the major types of optimization problems for continuous and discrete variable optimization, particularly nonlinear and mixed-integer nonlinear programming (MINLP). They have also reviewed the extensions of these methods to dynamic optimization and optimization under uncertainty. Their review paper [7] provides a general classification of mathematical optimization problems, followed by a matrix of applications that shows the areas in which these problems have been typically applied in process systems engineering. The important optimization methods used in chemical engineering fields are given in Table 1. In our opinion, it is hard to make generalized comments on the efficiency of the algorithms, but the characteristics of the mathematical model have a large influence on the choice of the solution methods.

Table 1. Overview of different solution methods for optimization of industrial processes.

Approach	References
Deterministic approaches	Biegler, L.T. & Grossmann, I.E. (2004). Retrospective on optimization. Computers & chemical engineering, 28(8), 1169–1192
Mixed integer non-linear (MINLP) - *Branch and Bound* - *Benders' decomposition* - *Outer-Approximation* - *Extended Cutting Plane*	Grossmann, I.E. & Kravanja, Z. (1995). Mixed-integer nonlinear programming techniques for process systems engineering.Computers & Chemical Engineering, V19, S1, 189–204 Gupta, O.K. & Ravindran, A. (1985). Branch and Bound Experiments in Convex Nonlinear Integer Programming. Management Science, 31 (12), 1533–1546 Kagan, N. & Adams, R.N. (1993). A Benders' decomposition approach to the multi-objective distribution planning problem. International Journal of Electrical Power and Energy Systems, 15 (5), 259–271.
Dynamic programming	Dadeboa, S.A. & Mcauley, K.B. (1995) Dynamic optimization of constrained chemical engineering problems using dynamic programming, Computers & Chemical Engineering, 19(5), 513–525
Meta-heuristic approaches	Jones, D. F., Mirrazavi, S. K., & Tamiz, M. (2002) Multi-objective meta-heuristics: An overview of the current state-of-the-art. European Journal of Operational Research, 137(1), 1–9.
Expert systems	Yamin, H.Y. (2004). Review on methods of generation scheduling in electric power systems. Electric Power Sys. Res., 69, (2-3), 227–248
Neural networks	Nascimento, C., Giudici, R., Guardani, R. (2000), Neural network based approach for optimization of industrial chemical processes. Computers & Chemical Engineering, 24 (9-10), 2303–2314
Genetic algorithms	Shopova, E.G. & Vaklieva-Bancheva, N.G. (2006). BASIC—A genetic algorithm for engineering problems solution. Computers and Chemical Engineering, 30, 1293–1309

Optimization problems encountered in process engineering need to address multiple objectives and often they are conflicting. A simple and the most common approach to solve such a multi-objective optimization problem (MOO) is to formulate a single aggregate objective function (AOF) by assigning appropriate weights with each objective based on the domain knowledge. This approach generally suggests a single trade-off solution rather than all possible trade-off solutions. Some of the recent advanced methods, which may be employed to seek solutions for various process engineering optimization problems, are listed in Table 2. For details regarding the evolution and importance of various methods, readers should refer to the respective references.

Table 2. Multi-objective optimization solution methods.

Multi-objective Optimization Solution Methods	**References**
Normal Boundary Intersection method	Vahidinasab, V. & Jadid, S. (2010). Normal boundary intersection method for suppliers' strategic bidding in electricity markets: An environmental/economic approach. Energy Conversion and Management, 51, 1111–1119.
Enhanced normalized normal constraint	Sanchis, J., Martínez, M., Blasco, X., &Salcedo, J.V. (2008). A new perspective on multiobjective optimization by enhanced normalized normal constraint method. Structural and Multidisciplinary Optimization, 36, 537–546
Successive Pareto Optimization method	Ancau, M. & Caizar, C. (2010), The computation of Pareto-optimal set in multicriterial optimization of rapid prototyping processes. Computers & Industrial Engineering, 58, 696–708
Multi-objective Optimization Evolutionary Algorithms	Tan, K.C., Lee, T.H. & Khor, E.F. (2002) Evolutionary Algorithms for Multi-Objective Optimization: Performance Assessments and Comparisons. Artificial Intelligence Review, 17, 253–290.
Genetic algorithms	Summanwar, V.S., Jayaraman, V.K., Kulkarni, B.D., Kusumakar, H.S., Gupta, K., & Rajesh, J. (2002). Solution of constrained optimization problems by multi-objective genetic algorithm. Computers and Chemical Engineering, 26 (10), 1481-1492
Non-dominated Sorting Genetic Algorithms	Inamdar, S.V., Gupta, S.K., & Saraf, D.N. (2004). Multi-objective Optimization of an Industrial Crude Distillation Unit Using the Elitist Non-Dominated Sorting Genetic Algorithm.Chem. Ind. Res. Des., 82(A5), 611–623
Strength Pareto Evolutionary Approach	Sarker,R., Liang, K., & Newton, C. (2002). New multiobjective evolutionary algorithm European Journal of Operational Research,1, 12–23
Chaotic Particle swarm optimization	Cai, J, Mab, X., Li,Q, Li, L., & Peng, H. (2009). A multi-objective chaotic particle swarm optimization for environmental/economic dispatch. Energy Conversion and Management, 50, 1318–1325
Simulated annealing algorithms	Suman, B. (2004). Study of simulated annealing based algorithms for multiobjective optimization of a constrained problem. Computers and Chemical Engineering, 28, 1849–1871
Analytic hierarchy process (AHP) and Goal Programming (GP)	Arunraj, N.S. & Maiti, J. (2010), Risk-based maintenance policy selection using AHP and goal programming. Safety Science, 48, 238–247

2.2. PSE Approach Towards Addressing Rising Environmental Concerns

In the last few decades the chemical process industries were looking for clean technological solutions [8] to minimize waste generation at the source rather than tackling it by using end-of-pipe treatment or remediation, not only because of the higher capital and operating cost associated with end-of-pipe treatment technologies, but also for better resource efficiency. Therefore, most of the methodologies for evaluating different process alternatives were restricted to specific problems, for example, minimization of waste materials, such as reaction byproducts, waste solvents, waste-water, vent losses, *etc*., or minimization of process water requirements. To understand the proposed solution methods, we discuss a few important methods and expert systems about the tools developed by the PSE community.

Alidi [9] has proposed a multi-objective planning model based on a goal-programming (GP) approach and the analytical hierarchy process (AHP), for the appropriate treatment and disposal of hazardous wastes generated by the petrochemical industry. He demonstrated the method with a hypothetical but representative example composed of two petrochemical plants, each generating two types of hazardous waste and one landfill site. The AHP provides an organized framework for systematically ranking goals relative to their overall importance, along with a variety of dimensions. AHP has been used to rank the priorities of the conflicting goals in the above example. Goal programming does not attempt to maximize or minimize a single objective function as does the linear programming model. Rather, it attempts to minimize the deviations among the desired goals and the actual results according to the priorities. The objective function of a goal programming model may be expressed in terms of the deviations from the target goals.

For the continuous plant, Halim and Srinivasan [10–12] presented a systematic methodology for waste-management and the intelligent system for the waste-minimization assessment. They proposed a methodology comprising three fundamental elements: process graph (P graph), cause-and-effect and functional knowledge. The P graph is a directed bipartite graph capable of abstracting the flow of materials in a process. An analysis based on the P graph provides a framework for diagnosing the origins of waste in the process and for deriving top-level waste minimization alternatives. These top-level alternatives can then be distilled further by using cause-and-effect and functional knowledge to obtain detailed alternatives. The application of the methodology is illustrated using an industrial case by the authors. In part 2, the authors proposed the architecture of ENVOPExpert, an expert system that implements this methodology. Given information concerning the process in the form of a flow sheet, process chemistry, and material information, ENVOPExpert can automatically detect the waste components in the process, diagnose the sources where they originate, and suggest intelligent design alternatives to eliminate or minimize them. In ENVOPExpert, waste minimization domain knowledge is organized into process-general waste minimization knowledge and process-specific information, whereas the inference engine contains algorithms for qualitative simulation, waste diagnosis, and alternatives generation, which use the process-specific information as a basis to perform the analysis. ENVOPExpert also assists the user to screen and rank the various alternatives using a waste minimization index. The application of ENVOPExpert to an industrial case study available in literature is illustrated, and the results obtained were found to be very close to the available experts' solutions. Batch processes in a multi-product manufacturing facility have always imposed numerous challenges

to the environment due to fluctuating loads. Recently, Halil and Srinivasan [13,14] have extended their work using an intelligent simulation-optimization framework for batch processes in a comprehensive sustainability analysis.

Karuppiah and Grossmann [15] used a superstructure approach for synthesizing an integrated water system comprising all process water as well as water treatment units. They have also shown the advantages of optimizing integrated networks by separate optimization of different sets of water using and treating operations. They have built a superstructure that incorporates all feasible design alternatives for water treatment, reuse and recycle and formulated the optimization of this structure as a non-convex Non-Linear Programming (NLP) problem. A new deterministic spatial branch and contract algorithm is proposed in which piecewise under- and over-estimators are used to approximate the non-convex terms in the original model to obtain a convex relaxation whose solution gives a lower bound on the global optimum. These lower bounds are made to converge to the solution within a branch and bound procedure.

The above papers cited in the literature discuss the usefulness of an expert system or a solution method in a given area of the process engineering. However, the sustainability studies are aimed at addressing the issues which are far beyond specific issues, such as waste-minimization or performance of a process. Therefore, for any sustainability assessment, it is logical to expand the boundaries of the existing process system or manufacturing unit to form a fairly large or more independent system or IEs.

2.3. Managing Complex Systems

Thus, the renewed chemical engineering approach [16] to the management of complex systems involving material and energy flows will be essential in meeting the challenges, mainly:

1. Combining ecological balance of an industrial system with their other goals of productivity and economic profitability.
2. Developing new operating model for industries

Improvements in understanding at the micro and molecular levels are always sought after, both for existing systems as well as systems being innovated. At the same time, the integration of this knowledge into "macro systems" is warranted to enable process engineering solutions addressing the sustainability framework [17]. The current ongoing efforts (discussed in next sections) are largely aimed at broadening the scope of "process optimization" to include new thoughts, factors arising out of the sustainability of the industrial eco system. These studies can be broadly viewed as those which addressed the various features of mathematical models and sustainability metrics which combine the conventional process plant models with the new constraints/goals, optimization techniques *etc*., individually and combinations thereof. The efforts, though nascent, have looked at several aspects of industrial ecological sustainability. Before we discuss the methods, we must first understand the philosophy of IEs through the prominent examples that appear in the literature.

There are many industrial ecoparks, industrial complexes and resource recovery parks being designed and developed across the globe with the support of local governments, non-governmental organizations, universities and research institutes, industries *etc*. These mainly originate based on the exchange of

resources between heavy industries in industrial complexes. These initiatives are generally referred to with the concepts of industrial symbiosis and eco-industrial parks [18]. We discuss five such examples in different parts of the globe:

(i) The industrial complex in Kalundburg, Denmark, is a famous example of IE [19]. This project was triggered in 1961 with the objective to save or minimize ground water for a new oil refinery. Now, it contains a power station, an oil refinery, a biotechnology company, a plasterboard producer, a soil remediation firm and a waste management company; exchanging various resources, including steam, water, gas, gypsum, fly ash, sludge, liquid fertilizer, *etc*. through a co-operative network and protocol developed local municipality [20]. In this industrial complex, different industries together formed a highly integrated industrial system that was optimized for the use of its byproducts in order to minimize the amount of net waste material or heat disposed of, resulting in substantial savings [21]. For example, the combination of heat and power production resulted in ~30% improvement of fuel utilization compared to a separate production of heat and power: using wastewater recycling the power plant has reduced water consumption by ~60%. The reduction in the use of ground water has been estimated at close to 2 million cubic meters per year.

(ii) A second example may be taken from Asian developing countries during recent years, where industrial ecology is emerging as a potential approach to reduce the environmental burden of rapid economic expansion [22]. Fang *et al*. [23] have studied industrial sustainability in China, where they described the Lubei industrial case. This ecosystem has 52 member enterprises and 5300 employees, with total assets of 5 billion yuan. Since 2001, the Lubei Group has been the largest producer of phosphate fertilizer in China as well as the largest manufacturer of ammonium phosphate, sulfuric acid and cement in the world. There are three major industrial value chains. The first comprises the industries which are producing ammonium phosphate–sulfuric acid–cement. The major focus of the second chain is integrated sea water utilization, mainly consisting of chemical process units producing salt, gypsum, potassium sulfate, magnesium chloride, bromine *etc*. The third is a salt–alkali–electricity manufacturing chain. The Lubei integrated industrial system reveals synergy in the re-use of by-products, both within and among the three production chains. Sulfuric acid and seawater are the basic material flows, steam and electricity are the energy flows, and gypsum and furnace slag are the main "waste" flows. Fang *et al*. [23] also reviewed the sustainable development created by promoting a circular economy (CE) with optimal utilization of resources and energy; and maximization of integrated community profit.

(iii) Heeres *et al*. [24] compared IE systems in The Netherlands and in the US and found that Dutch EIP projects are more successful in their initial development than the US cases. Although most of the projects were in the early stages, the initial success of the Dutch projects was attributed to two factors, the first being the active participation of companies in the project. This may be addressed by an association of the local entrepreneurs, which could be an effective platform to educate and inform companies of the potential benefits that can be achieved through the establishment of an IE. The second factor is the willingness to share the costs of EIP planning by companies. Participating companies should also be financially committed rather than depending on the

government to fund such initiatives. This would help to ensure the commitment of the participating companies in the later phases of the program.

(iv) The Synergy Industrial Park at Carole Park is an important initiative by the Queensland government and private sector partners in demonstrating the application of industrial ecology in Australia. The important lesson learned from the Synergy Park project is the need to engage business and the community in a program of education to support eco-industrial development [25].

(v) In the US, the Mississippi River Corridor Industrial Complex comprises around 150 chemical plants. Research activities are in progress to minimize waste disposal and maximize material and energy reuse in such complexes [26].

As can be seen from these five examples, industrial ecosystems are those in which the utilization of various natural resources is maximized and waste generation minimized. The effort is to ensure that even as we address the growing needs of societies, we employ methods which will minimize the irrevocable damage done to nature. This leads us to view the industrial ecosystem as broadly as possible to include all the units and entities with which a given process industry exchanges mass and energy. This understanding therefore brings into focus not only the productivity of an industry, the waste generation, and effect on the immediate community (environment), but also the effect of the finished goods through their life cycles. The sweep of sustaining such a system is dauntingly large. To make it sustainability more manageable, we look at the efforts that have already been made in the next section.

3. Sustainability Assessment of an IE

As industries are realizing the importance of sustainability principles while making business designs, it is expected that sustainability indicators are easy to formulate. In addition, their utility in influencing various decisions must be clearly established, not only at the process level but also in the corporate balance-sheet and society. There are three major aspects of sustainability indicators, mainly economic, environmental and social [27]. The fourth aspect, institutional dimension proposals [28] are still quite rare. The economic indicators are mainly NPV (net present value), cash-flow after tax, research expenditure and fines. Environmental performance indicators mainly deal with hazardous waste, emissions and spills where social aspects take into account social and community investments, accident rates, injury frequency and fatalities. In this section we firstly describe briefly the environmental indicators currently being used in the industry and then discuss improved models for the environmental assessment which are within the scope of PSE.

3.1. Environmental Performance Indicators

There is a strong influence of environmental indicators on environmental management and policy-making at all levels of decision-making. However, the scientific basis of the selection process of the indicators used in environmental reporting can be significantly improved [29]. Life cycle assessment (LCA) is considered to be a systematic approach to evaluate the environmental burdens caused by a material, a product, a process, or a service throughout its lifespan. Information from an LCA can be used to assess design options for a given product or a manufacturing process, or it can be used for comparing different products for the same application. In general, there are two kinds of LCA

methods available that can generate one single score for every product. The first type of indicator analyzes all potential environmental impacts occurring during the life cycle, whereas the second type generates input-related indicators [30]. The first type of methods are quite common in practice, such as Ecoindicator 99 [31], which accounts for the depletion of non-renewable resources and various impacts resulting from a chosen manufacturing process and the use of the products under consideration. A single score per product may be obtained by applying appropriate weighting factors. The LCA approach, typically followed by a sustainability analysis, mainly relies on the database established in different impact or damage categories, such as global warming potential, carcinogenic effect *etc*. The LCA method can provide a comparative analysis of different design schemes of an industrial ecosystem to evaluate the corresponding environmental impacts. However, this analysis is still not able [32,33] to account for all ecological products and services, mainly due to following issues:

(i) Higher degree of uncertainty or lack of data in the impact assessment of various categories, such as global warming, ozone depletion, eco-toxicity, human toxicity *etc*. We believe that the majority of these are due to the lack of a quantitative assessment of ecological processes and the impact of their emissions.

(ii) Difficulty in the traceability or quantification of some of the streams or species. This is mainly due to the fact that the ecological system boundaries are not well established or understood, and also that these streams or species are not included in the economic analysis, as the industrial system does not pay a price to these, hence, the go unaccounted.

(iii) Not all types of impacts are equally well covered in a typical LCA. For example, assessment of land use, including impacts on biodiversity and resource aspects, including freshwater resources, are problematic and need significant improvement.

In our opinion, some of these may never be solved completely, but a comprehensive assessment methodology is required which would encompass the principles of process economics, environmental systems and ecological systems. This may help to understand and address the complexity and impact. However, the more versatile input-output modeling approach and the extension of the same, is discussed below. This will possibly help to establish the relationship of various products and services in an IE with the performance parameters.

3.2. Input-Output Analysis (IOA)

This approach was familiar in the macro-economic study of the monetary flows through various economic sectors, but recently it was applied to the industrial systems to model the material and energy flows in environmental impact analysis by Bailey *et al*. [34]. In this modeling approach, source and destination of each material or energy flow in a given industrial system at a given point in time are tracked, and a mathematical framework considers direct and indirect relationships among conserved flows. If the mathematical expressions derived from an ecological standpoint or for an eco-system are included, it is known as Ecological Input-Output Analysis (EIOA). EIOA may be considered as an "all-inclusive model" for the assessment of an IE because of its ability to capture the economics, environmental, and societal behavior of an IE. Also, it could be utilized to illustrate the detailed

inter-relationships among the entities in an IE. Bailey and coworkers have developed a tool called "environ analysis" for considering all direct and indirect paths taken by material or energy flows through an industrial system. A typical EIOA consists of the analysis of a system's nodes and flows, where a node represents any processing unit, industrial entity, or individual subsystem of interest and a flow characterizes an interested material, energy, or other conservative input and output from a node. The EIOA presented by Bailey and co-workers does not differentiate between waste and product output from a node; rather, all outputs from the system are lumped into a single term. Accountability of various streams, and, hence, ultimately ecological products and services, would be a lot easier if there is a distinction between a consumer product and a waste to the environment. Piluso *et al*. [35] have further modified EIOA by making a provision to distinguish between consumer product and environmental waste. However, the authors have not illustrated the optimization of a network to achieve the optimal design with regard to the "triple bottom lines" (economic, environmental and social aspects) of sustainability. Also, this methodology relies on the end-users to provide potential network modifications. As there are various conflicting objectives, multi-objective optimization techniques are often employed to tackle such an optimization problem. Some of the challenges not yet encountered by the scientific community for employing such multi-objective optimization techniques for ecological studies involving commercial chemical plants are discussed in the next section.

3.3. Challenges with "LCA-Centered Optimization" and Traditional Optimization Tools for IEs

The major objective of any industrial system is to determine the configuration of an entire network with the goal of maximizing the economic performance and minimizing the environmental, health and safety impact. The decisions that should be made include the technologies to be installed in the plants, the capacity or production rates and location of the plants, and warehouses for raw materials and products. To solve such complex optimization problems, the general approach cited in the literature is to formulate a large-scale mixed integer program which includes all supply-chain associated units. Various traditional optimization strategies mentioned in Section 2.1 may be employed. Hugo and Pistikopoulos [36] have described a methodology for environmental impact minimization by using a generic mathematical programming model to assist strategic long-term planning and the design of chemical supply chain networks. They have combined the classical features of the capacitated plant location problem with the concept of LCA and multi-enterprise supply chain management. A mathematical programming-based methodology was used for the explicit inclusion of LCA criteria as part of the strategic investment decisions related to the design and planning of supply chain networks. By considering the multiple environmental concerns together with the traditional economic criteria, the planning task was formulated as a multi-objective optimization problem. Over a long-range planning horizon, the methodology utilizes mixed integer modeling techniques to address strategic decisions involving the selection, allocation and capacity expansion of processing technologies and the assignment of transportation links required to satisfy the demands of the markets. At the operational level, optimal production profiles and flows of material between various components within the supply chain were determined. The solution to this kind of problem is known as the set of efficient or Pareto optimal solutions. A similar approach was also proposed by Guillen-Gosalbez & Grossmann [37] and Gebreslassie *et al*. [38].

For an IE, while the boundaries of an industrial process are expanded further, multi-objective optimization involving economic performance and environmental performance using conventional LCA approach is complex. For example, it may not be practical to integrate LCA tools with the existing ERP (enterprise resource planning) tools or process modeling tools typically used by financial analysts or process engineers in various industries. Also, there are uncertainties with LCA as discussed in the previous section, which makes the optimization further complicated. Hence, the sustainability assessment tools, in the form of sustainability indicators, which are easy to formulate and interpret by different users across the industrial eco-system, would be beneficial. Therefore, in the next section we discuss the simplified form of sustainability indicators available in the literature which are based on embodied energy concept.

3.4. Sustainability Assessment of An IE Using Embodied Energy

The growth potential of an IE is estimated not only based on the availability of energy, both in terms of quality and quantity, but also its capacity to convert it to useful work. As we move higher in the value chain of products or fuels [39], the quality of energy is improved but the quantity may be substantially reduced. For example, the useful energy per unit mass of the final product such as bio-ethanol or bio-diesel could be lot higher than its bio-mass source. The ecological cost of nature's products and services may be estimated as the amount of energy used directly or indirectly in its manufacture, which is called emergy [40]. Thus, emergy is the embodied energy or energy memory in any product or service. For convenience, various energy units can be simplified by converting them into a common unit of solar energy. Odum proposed a concept of Solar emergy which is the amount of solar energy used directly or indirectly to make a product or service. Solar emergy is measured in solar: transformity [41] is derived. Transformity is defined as the emergy of one kind of available energy required to make 1 joule of energy of another type. The unit of transformity is "solar emjoule per joule" as the emergy can be calculated in terms of solar energy. In some cases where the transformity is not known, the emergy to money ratio is used in estimating the emergy of the products or the services. For example, Emdollars, can be calculated by dividing the total emergy use of a country by its gross economic product. A detailed example of the emergy evaluation and its application to a complex system is illustrated by Wang *et al*. [42] for an eco-industrial park.

The Emergy analysis helps to express the economic values and environmental factors in a generalized mathematical form. It also provides a common platform for the comparison of the economic and environmental status of different units. Thus, the sustainability performance of the ecosystem could be assessed using a set of emergy-based indices proposed by several researchers. Earlier emergy-based sustainability indices reported in the literature, [43] and Brown & Herendeen [44], were developed from the study of agricultural or natural ecological systems and the new indices are devised by addressing the unique features of industrial systems, *i.e*., waste treatment, recovery, reuse and recycling, while considering all of the material/energy flows and investments in industrial systems. The applicability and effectiveness of the emergy-based indices in analyzing industrial systems can be improved significantly. Lou *et al*. [45] have introduced a set of indices to quantitatively assess the environmental and economic performances as well as the sustainability of industrial systems. These indices are as follows:

(i) Index of Economic Performance (IEcP): This index is the ratio the sum of the emergy of the main product and byproduct and the yield generated from waste, divided by the emergy of the total investment to obtain the required quantity and quality of the product while satisfying environmental regulations. A process can be made profitable by maximizing the production while minimizing the total investment.

(ii) Index of Environmental Performance: The index of environmental performance (IEvP) is the ratio of the sum of the emergy of non-renewable resources consumed and the waste disposed of into the environment, with or without treatment, during the production process to the total emergy of the renewable resources used in the process and the internal recycle streams for renewable and non-renewable resources generated from treated as well as untreated waste. A low value of IEvP is always desirable, because it indicates less pressure on the environment. The value of IEvP can be improved by replacing non-renewable resources with appropriate renewable resources. Implementing the internal recycling of waste as renewable or non-renewable resources can also largely reduce the value of the IEvP.

(iii) Index of Sustainable Performance: The index of sustainable performance (ISP) is the ratio of IEcP and IEvP. It is a measure of the overall sustainability of a process, because it combines the economic as well as the environmental performance of a process.

The above-mentioned indices are more comprehensive, which could potentially quantify the realistic value of all the resources, services, and commodities irrespective the financial value, and could be easily applied to a wide range of industries. It is expected that the sustainability must consider economic performance and environmental stress simultaneously; hence, it is more appropriate to use both the IEcP as well as the IEvP explicitly to evaluate the overall performance rather than using ISP alone.

It is not only important to know the cumulative environmental impact of an IE but there is also a need to understand the contribution of an individual unit and the relationship between various units from the sustainability viewpoint. This would allow one to identify opportunities to improve the overall sustainability of an IE while protecting economic interests of the individual units. Cao and Feng [46] have shown that the emergy indices of an IE can be expressed as the sum of distribution of emergy indices (DEI) of individual units, whereas DEI is equal to the product of the weighing coefficient of a unit and the corresponding emergy index. The weighing coefficient generally corresponds to the fraction by which it affects the IE. This analysis could be imperative to solve the complex multi-objective or multi-criteria optimization problem.

4. Simplified Approach for Optimization of an IE

For a larger size chemical process network, existing optimization algorithms may not deal efficiently with such complex problems. Computational issues/difficulties could arise, mainly due to highly non-linear functions, a large number of variables and the interactions among these variables. To solve such complex problems, it is generally preferred to structure the complex optimization problem using principles of hierarchical decomposition as illustrated by Zondervan *et al*. [47]. In this approach, an industrial system is viewed as having multiple levels of decision-making. As a complex system is separated into several independent sub-systems at different hierarchy levels, the complex optimization

problem is also separated into several sub-problems which have fewer variables and simplified functions. Such simplified independent problems could be solved using conventional optimization techniques. These independent sub-systems are then coupled through variables which could be manipulated at a higher level to obtain an optimal solution for a given larger industrial system.

From the discussion in the previous section, it is evident that maximum sustainability could be obtained at maximum IEcP and minimum IEvP. Therefore, it is necessary to formulate the optimization problem as a multi-objective optimization (MOO) problem at a higher level in the hierarchy. In such cases, generally it is challenging for decision-makers to arrive at a solution that provides them with the best values simultaneously for all criteria and often a trade-off is essential. For example, in the Pareto optimality concept, a solution of a MOO problem is considered Pareto optimal, if there are no other solutions that better satisfy all the objectives simultaneously. This is called non-inferiority. Solution methods for generating the Pareto front are broadly divided in two classes [48]. One class of solution methods is deterministic in nature. Examples are (i) weighted-sum; (ii) normal boundary intersection; (iii) normalized normal constraint *etc*. They generally transform the MOO problem into a series of single objective optimization problems and Pareto-set is obtained by varying the parameters of the method employed. The other classes of methods are population-based stochastic methods, such as evolutionary algorithms and particle swarm optimization, which are capable of finding solutions much quicker for the complex optimization problem.

It is expected that applying hierarchical decomposition along with the MOO solution method would make the optimization of a larger system manageable. The hierarchical-Pareto optimization methodology proposed by Singh and Lou [49] is one such plausible hybrid technique where a linear weight method is used to generate the Pareto frontier. In their work, they have illustrated how the maximum sustainability of an IE could be obtained for a given plant size under normal operations. Typically, in a given IE in a lower level of hierarchy, individual economic and environmental objectives of each individual industry are identified independent of the objectives of the other industries in an IE. At the upper level, the optimization algorithm calculates the overall objectives of the entire IE, *i.e.*, to maximize the overall economic performance and minimize the environmental pressure and eventually maximize the overall sustainability of the entire ecosystem. In their study, very little emphasis is given to understanding and resolving the typical problems encountered by the participating industries due to the uncertainties or improving flexibility of an individual industry. Robustness of the network is essential from an overall sustainability standpoint. The robust optimization of chemical processes is a key to the success of the entire network. Developing an optimization framework for an individual industry is fairly complex. Essentially, a lower level, *i.e.*, individual industry model, requires further decomposition.

5. Robust Optimization of Chemical Processes

There are possibilities of process upsets or unplanned shut-downs experienced in chemical process plants which disturb the production planning and scheduling for that industry, and as a result other units of IEs may experience some pressure or short-supply. To avoid such a situation, a general tendency of the industries is to over-design the critical units. This over-design can potentially affect the economic performance index. There have been few attempts to address the uncertainties at different

levels and on different time scales. Diwekar [50–52] has combined AI approaches with optimization methods while using the system constraints based on thermodynamics and physics and extended traditional process design framework to green process design and industrial ecology, leading to sustainability. For this purpose, Diwekar proposed a multi-layer (five layers) algorithmic framework in order to simplify complex optimization problems, as discussed in the next paragraph.

The innermost layer (layer-5) corresponds to models for process simulation, thus capturing the thermodynamics and physics of the problem. This would essentially capture possible chemical and process alternatives for a particular process. This may be formulated using conventional tools, such as Aspen Plus. Layer-4 is considered as sampling loop, which deals with the diverse nature of uncertainty, such as estimation errors and process variations, and can be specified in terms of probability distributions. In layer-3 the objective function is formulated using only continuous variables, such as process conditions, whereas discrete variables are separately dealt with in layer-2, which is the most difficult to handle due to the discrete decision variables. The outermost layer (layer-1) is a large array of analytical techniques to solve the multi-objective optimization problem which could be either the preference based methods for example goal programming or the generating methods which result in pareto optimal solutions.

Diwekar's work, discussed above, reveals that for real world large-scale combinatorial problems, stochastic programming solutions are more promising compared to the deterministic solution, and that stochastic annealing algorithms are recommended to optimize any probabilistic objective function. In the stochastic annealing algorithm, the optimizer not only obtains the decision variables but also the number of samples required for the stochastic model, which may be also used for a trade-off between accuracy and efficiency. Having a set of representative samples from the multivariate probability distribution is critical in measuring performance statistics. Diwekar's approach of using the quasi-Monte Carlo scheme, such as a Hammersley sequence sampling which gives more uniform samples for a multivariate probability distribution, was found to improve the computational efficiency of the stochastic annealing framework. This research group has used this algorithmic framework for synthesizing a power plant and design of a separation process in two separate case studies. However, they did not discuss the utility of sustainability indicators in their decision-making processes. However, the optimization philosophy presented by Diwekar may provide a way to address the issues arising due to uncertainties for a large size chemical process plant.

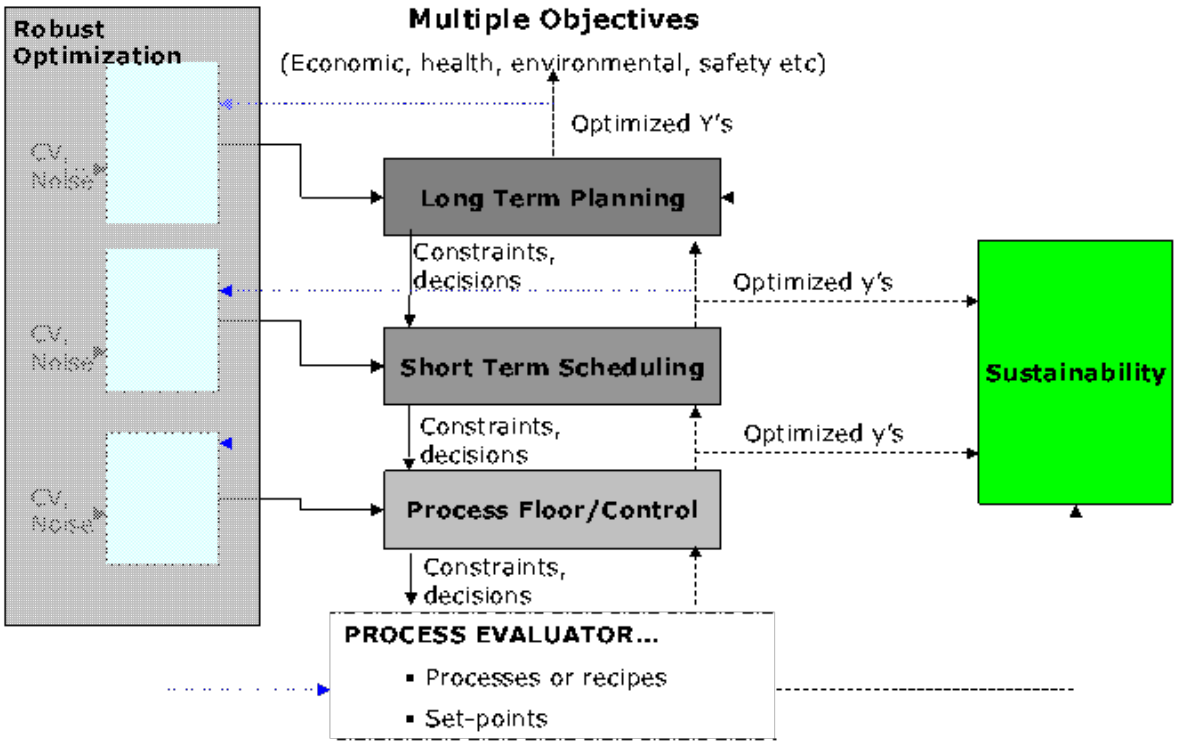
In another approach to simplify the optimization of steady-state chemical processes, the use of less complex metamodels or surrogate models is suggested [53–55]. This technique is often used by mechanical engineers or structural engineers while dealing with optimization involving complex finite element method (FEM) simulations. Such FEM simulations could be time-consuming or there may be the risk of an optimization program being confined in the local optima. Metamodels establish the relationship between design parameters and response parameters.

6. Towards Robust Optimization of An IE

Economic and environmental sustainability are achieved through the optimal use of renewable feedstock, and a need exists for a PSE approach to ensure maximum economic and societal benefit through minimizing the use of raw material and energy resources as well as the cost involved in supply

chain operations [56]. Also, the robustness assessment or robust optimization of fully integrated industrial systems (or IE) is not explicitly addressed in the references given in the earlier sections. In our opinion, success in obtaining a reliable and optimal solution for a sustainability of a given IE lies in decomposing the complex system into various sub-systems, integrating the sub-systems through coupling variables, selecting the appropriate mathematical programming and optimization techniques to solve individual sub-problems as well as selecting appropriate process intensification techniques. Essentially, a large size IE comprising many industries could have two levels (as explained in Section 4). But at an individual industry level, further hierarchical decomposition is looked for to address uncertainties associated with the individual processes or other operations in a given industry. A multi-level framework is more frequently used [57–59] for an individual process industry rather than a single level. At the uppermost level of an individual industry, planning is based on current and future market demands. In the middle level, detailed scheduling over a short-term time horizon is generally considered, whereas in the bottom level, individual processes are considered in detail for individual products or intermediates. This three-level hierarchical framework could be coupled with two independent blocks which would perform sustainability analysis as well as robust optimization as shown in Figure 2 for an individual industry. The constraints and decisions may be imposed from other layers, whereas the values of control variables (CV) are optimized locally using a suitable optimization solution method, this would probably improve the efficiency. The decisions taken at the individual level regarding the optimized parameters and the respective value of the objective functions (y's) are further communicated to the other blocks and thus the optimization may be performed from the bottom to the top. This process could be iterative, if the feedback loop is established. Essentially, Figure 2 shows the hierarchical decomposition of an individual industry, which may be able to address the issues arising due to uncertainties as well as help to improve the flexibility of an individual industry. Further, this proposed multi-level robustness assessment or robust optimization philosophy of an individual industry may be translated to the two level IE model proposed by Singh and Lou [49]. The major advantage of this methodology is that it conceptually simplifies the complex system and modularizes each individual subsystem. But because of the decomposition of a monolithic problem into several sub-problems, we may encounter a higher error in the model predictions or lose the focus on the global optimality. In order to overcome this problem, it is necessary to build high fidelity models and improve communication between various levels, as well as establish feedback mechanisms which would help to improve the effectiveness of the method. Metamodeling techniques look promising when such hierarchical decomposition is attempted.

Figure 2. Proposed framework to assess the robustness of an industrial system.



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