Transactions National Academy of Science & Technology Philippines
ISSN 0115-8848 (print)
ISSN 2815-2042 (online)

Vol. 40 No. 2 (2018)

doi.org/10.57043/transnastphl.2018.1088

Optimizing Resource Conservation Networks: Overcoming Barriers with Process Systems Engineering

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ABSTRACT

Climate change continues to be the major environmental challenge of this century. Some of its effects may include more severe weather conditions, increased incidence of water scarcity, and the potential of pandemic outbreaks, to name a few. Scientific research has thus looked into various strategies to address this problem. These include reducing the generation of greenhouse gas emissions (GHGs) through the implementation of low carbon technologies and transitioning towards a more circular economy through improved resource efficiency. The challenge is in identifying which among the available options would yield the best results. The field of process systems engineering (PSE) which is a computational branch of chemical engineering, provides rigorous methods for analyzing systems which can be used to support decision making. These methodologies have been implemented at various scales to identify strategies which can improve the environmental performance of industrial systems. It has been utilized for optimizing operations of industrial processes, managing resources in eco-industrial parks, greening the product supply chain, and even analyzing strategies for reducing national carbon emissions. This work provides an overview of how PSE tools can be utilized for the design of more sustainable systems and showcases how it can be used at various levels of implementation.

Keywords:
process systems engineering, circular economy, mathematical optimization, climate action

Citation:
Aviso KB. 2018. Optimizing resource conservation networks: Overcoming barriers with process systems engineering. Transactions NAST PHL 40 (2): doi.org/10.57043/transnastphl.2018.1088

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Plenary paper presented during the 40th Annual Scientific Meeting (July 2018) of the National Academy of Science and Technology Philippines.

INTRODUCTION

Climate change is the single most important environmental issue of this century. It is expected to bring about more severe weather conditions, increased incidence of water scarcity, and even the outbreak of pandemics. In 2009, Rockström and colleagues (Rockström et al. 2009) identified key indicators which are necessary for human survival in earth together with their recommended levels for sustainability. Freshwater use and atmospheric CO_2 concentration are among these indicators. In 2016, the atmospheric CO_2 concentration had already exceeded the recommended level of 400 ppm (Jones 2017) while accounting for global freshwater use needs to be examined more closely to achieve a more accurate measurement (Jaramillo and Destouni 2015). Because of this, various strategies are being explored to improve the environmental performance of industrial processes and the best option is to implement multiple strategies simultaneously.

Improving energy use efficiency can potentially contribute more than 50% of the required

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reduction in carbon emissions, use of renewable energy by 20%, and carbon capture and storage by another 20% (Pacala and Socolow 2004). More recently, it has been suggested that more innovative technologies such as negative emissions technologies will be needed to meet net zero carbon emissions by 2050 (Haszeldine et al. 2018). The selection of the most adequate mix of technology options to implement and the level by which to implement them requires a systematic framework which accounts for interdependencies in the system being considered. The field of industrial ecology (Ayres and Ayres 2002) and the concept of circular economy (Kalmykova et al. 2018), for example, intend to transform the linear flow of materials and energy into a more circular one. In this regard, tools such as Life Cycle Assessment (Guinee 2002), which quantifies the environmental impact of products and services along the product life cycle, and input-output analysis (Leontief 1936) which provides a framework for modelling interdependencies between system components, will be needed to design more sustainable industrial systems. Furthermore, the field of process systems engineering (Stephanopoulos and Reklaitis 2011) provides rigorous methods for the design and synthesis of processes in industrial plants and can be extended for application to industrial clusters, enterprise models, and even regional or national economic systems.

This work provides an overview of how PSE tools together with sustainability concepts can be utilized for the design of more sustainable industrial systems. The rest of the paper is organized as follows: (a) the formal problem statement; (b) discussion of the different sustainability concepts and modelling frameworks which can be used for the analysis of industrial systems; (c) case studies on how these methods have been utilized at various levels of the industrial system as tools for design and analysis; and (d) conclusions and recommendations for future work.

PROBLEM STATEMENT

The formal problem statement can be defined as follows:

- Given an industrial system which consists of N number of components
- Given that the operation of the industrial system is needed to generate P number of goods or services
- Given that the operation of the industrial system is accompanied with M number of environmental emissions
- Given that there are several options to improve the environmental impact of the industrial system

The problem is to identify the optimal operating condition of the industrial system and the selection of the appropriate mix of strategies to achieve the best environmental performance of the system.

Industrial Ecology and Circular Economy

The flow of materials within the industrial system used to follow a linear path where resources are extracted from the natural environment, utilized, processed, and finally disposed off as waste. This occurred when people thought that resources were unlimited and that the environment can assimilate all the waste that was disposed. However, the realization that natural resources are limited and that the disposal of waste affected the environment, resulted in the promotion of waste management strategies beginning with pollution control technologies. Now, the objective is to transition towards a more circular flow of materials and energy through the promotion of cleaner production, sustainable consumption, and source reduction schemes.

This concept was initially introduced by Frosch and Gallopoulos (1989) and became the foundation of the principles of industrial ecology (IE). The distinguishing feature of IE is the identification of processes occurring in natural ecosystems which can be adopted to make industrial systems more sustainable. The two main concepts are industrial symbiosis and industrial metabolism. Industrial symbiosis is patterned after natural symbiotic relationships which occur in biological ecosystems. The concept is to identify how waste materials from

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one industry can potentially be used as raw material for another, thereby reducing the consumption of virgin resources and the generation of wastes. One of the most famous examples is the eco-industrial park of Kalundborg, Denmark (Jacobsen 2006) where companies co-located within the same region developed a network for material and energy exchange to reduce virgin resource consumption and waste generation.

Industrial metabolism, on the other hand, is more concerned with how materials and energy flow through industrial systems. It looks at how efficiently resources are utilized, where resources are sourced from, and where they eventually end up in. The intention is to improve the utilization of resources where economic growth can be sustained even with reduced input of materials.

Input-Output Analysis

Input-Output Analysis (IOA) was developed by Leontief (1936) to describe the interdependence between economic sectors. The economic system may be represented as a system of interacting components as shown in Figure 1 where each economic sector not only utilizes inputs from other sectors to perform its function but also provides services and products which can be utilized by other sectors. IOA models were utilized to analyze how economic shocks impact the economy.

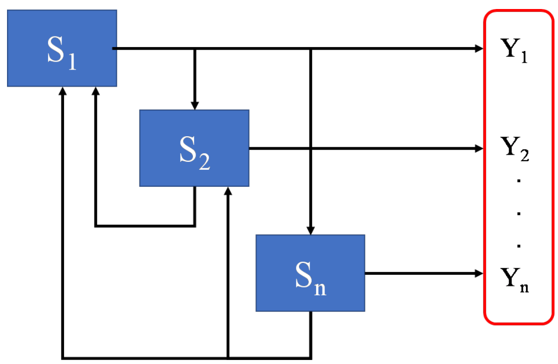

Figure 1. Representation of an economic system.

The basic equation is as indicated in Eq. 1 where **A** is the coefficient matrix which contains elements a_{ij} indicating the proportion of input from sector *i* needed by sector **j** to generate a unit of output; **x** is the total output vector which indicates the size of the economic sectors and **y** is the net demand vector. It can be rewritten into Eq. 2, where **I** is an identity matrix having the same size as matrix **A**. Thus, given the desired demand vector for an economic system, it is possible to solve for the required system size using Eq. 3. The total output vector accounts for the internal requirements within the economic system together with the final demand needed. The interested reader is directed to the work of Miller and Blair (2009) for more details.

Though initially used for accounting both direct and indirect impact of economic shocks, IO models have been extended for analyzing inoperabilities (Haimes and Jiang 2001), integrating environmental impact into economic systems (Heijungs and Suh 2002), modelling supply chains (Albino and Kuhtz 2004), and even for examining the interactions within organizational systems (Correa and Parker 2005). A recent book by Tan et al. (2019) discusses the applications of the IO model for various sustainability issues. It provides a framework for modelling interdependence within systems.

$$\mathbf{Ax} + \mathbf{y} = \mathbf{x} \quad (1)$$

$$(\mathbf{I} - \mathbf{A})\mathbf{x} = \mathbf{y} \quad (2)$$

$$\mathbf{x} = (\mathbf{I} - \mathbf{A})^{-1}\mathbf{y} \quad (3)$$

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Life Cycle Assessment

Life Cycle Assessment (LCA) is a framework for quantifying the environmental impact of products and processes throughout their life cycle. This includes accounting for material, energy, and environmental emissions from raw material acquisition, material processing, transport, manufacture, use, and end of life disposal and management. This provides a more holistic examination of the environmental performance of products by not just focusing on the environmental impacts associated with product manufacture and use. Similar with economic systems, life cycle phases are interconnected with each other and thus may be modelled using the IO framework (Heijungs and Suh 2002). The different phases involved in conducting LCA is shown in Figure 2. The goal and scope definition phase is meant to set the objectives of conducting the LCA, identifying key assumptions, data requirements, system boundaries, and the unit of assessment or functional unit.

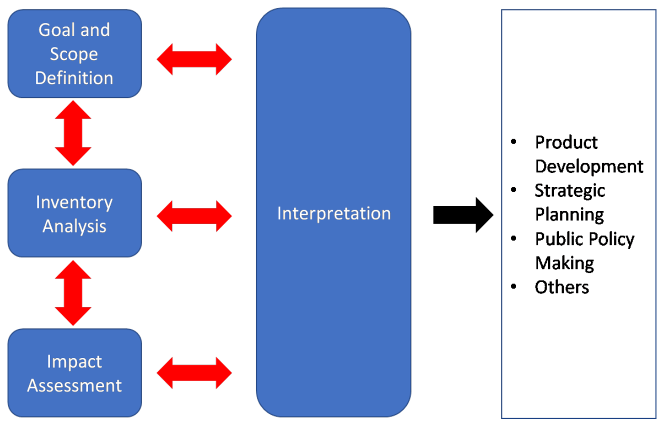

Figure 2. Phases of Life Cycle Assessment (adopted from ISO 14040 1997).

The inventory analysis phase is meant to quantify all material and energy flows in the system. This includes both economic and environmental elements in the system. The matrix based LCA provides a framework for adequately scaling the flow of streams from individual processes into the desired size or capacity of the system based on the identified functional unit. The inventory is calculated using Eq. 4 where matrix **A** is an *n* x *n* technical coefficient matrix which indicates the flow of streams between processes in the system; **s** is the scaling vector which dictates the magnitude by which processes should be scaled in order to meet material and energy balances in the system; while **f** is the functional unit vector which contains the basis by which the accounting is being made. Both matrix **A** and vector **f** are typically defined with vector s being the unknown variable. Vector **s** can be solved using Eq. 5.

$$\mathbf{As} = \mathbf{f} \quad (4)$$

$$\mathbf{s} = \mathbf{A}^{-1}\mathbf{f} \quad (5)$$

Each process considered in the process will also have an associated environmental impact. This is accounted for in the *m* x *n* intervention matrix **B** such that the total environmental inventory vector **g** can be obtained using Eq. 6 or 7. The environmental emissions are then categorized based on the nature by which they affect the environment. This is done in the impact assessment phase (Figure 2). Translating the environmental inventories into the corresponding environmental impact is done using Eq. 8 where **Q** is the characterization matrix and **h** is the environmental impact vector. The interested reader is directed to the work of Heijungs and Suh (2002) for a more detailed discussion of the calculations.

$$\mathbf{Bs} = \mathbf{g} \quad (6)$$

$$\mathbf{BA}^{-1}\mathbf{f} = \mathbf{g} \quad (7)$$

$$\mathbf{Qg} = \mathbf{h} \quad (8)$$

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Process Systems Engineering

Process systems engineering (PSE) is a branch of chemical engineering which provides a rigorous framework for analyzing system structures (Stephanopoulos and Reklaitis 2011). It is concerned with the interaction of system components and how these interactions affect the over-all behavior of the system. It has been utilized for various applications including process design and synthesis, optimal process scheduling and planning, and mathematical optimization and simulation to name a few. Its application to sustainability issues have also recently gained wide interest and attention among the chemical engineering community. One of the earliest applications of PSE was in the development of the Solvay process which resulted in the creation of new integrated processes in order to achieve higher process yields, reduced waste generation, and improved economic costs (Stephanopoulos and Reklaitis 2011). At the core of PSE are the principles of material recycling and energy integration in order to improve process efficiencies. These principles are the same concepts which should be applied in transforming linear industrial systems into more circular ones. The tools and techniques implemented in PSE can thus be exploited and implemented at various levels in order to create more sustainable industrial systems.

Resource Conservation Networks between Multiple Industrial Plants

The principle of resource conservation networks may be implemented for industrial plants which are co-located within the same region similar to an eco-industrial park. Keckler and Allen (1998) proposed a methodology for water re-use in an industrial park. The goal is to identify the network design which will minimize the total resource consumed within the system (e.g., minimize freshwater use) and this is just the summation of the individual freshwater flowrates consumed by each plant *j* (F_j) in the industrial park as shown in Eq. 9. This however can also be implemented for other types of resources. The development of the optimal network is subject to material balances from available water sources *i* (Eq. 10) and receiving water sinks *j* (Eq. 11) where R_{ij} represents the flowrate of the resource exchanged from source *i* to sink *j*; W_i is the excess resource from source *i* which ends up as waste; S_i is the total amount of resource from source *i* and D_j is the amount of resource needed by sink *j*. Furthermore, the exchange of resources should meet any quality considerations or requirements in the receiving industrial plant represented by the quality indicator, Q_j. This constraint is shown in Eq. 12 where C_i represents the quality indicator characteristic of source *i* and C_F the quality characteristic of the fresh resource. The schematic diagram of this process is shown in Figure 3 where a network will be established between industrial plants that initially operated independently of each other.

$$\text{Min} = \sum_{j=1}^{N} F_j \qquad (9)$$

$$\sum_{j=1}^{N} R_{ij} + W_i = S_i \qquad (10)$$

$$\sum_{i=1}^{M} R_{ij} + F_j = D_j \qquad (11)$$

$$\sum_{i=1}^{M} R_{ij}C_i + F_jC_F \le D_jQ_j \qquad (12)$$

The methodologies such as the model presented above were extended and improved to account for multiple stakeholder objectives. The satisfaction of these objectives becomes critical if cooperation between the network participants is desired. Aviso et al. (2010a) developed a fuzzy optimization model for water re-use in an eco-industrial park. Further, Aviso et al. (2010a) utilized max-min aggregation and the fuzzy membership function to integrate the multiple objectives into a single satisfaction objective (Eq. 13) which is normalized to have a value from 0 to 1 (Eq. 14). The degree of satisfaction is a linear function which follows Eq. 15 for parameters which need to be maximized or Eq. 16 for those that should be minimized. This framework was later on modified to account for the presence

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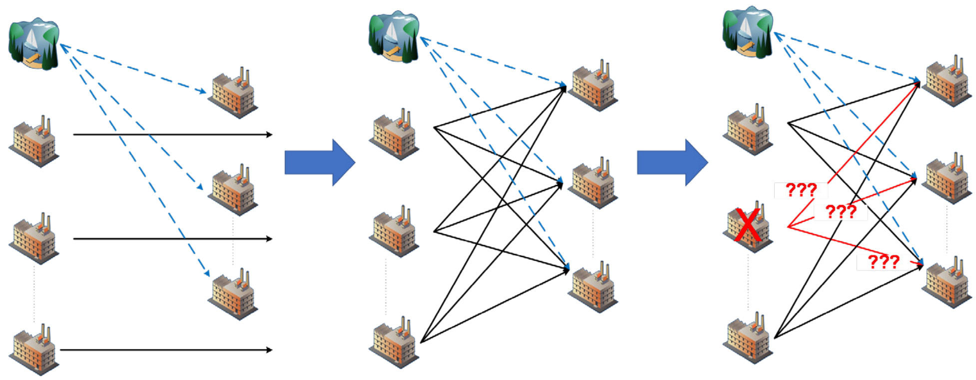

Figure 3. Schematic Diagram of Resource Conservation Networks.

of stakeholders which might not have the same level of influence on the solution. Such cases occur between a park authority and the park tenants. A leader-follower strategy similar to a Stackelberg game is then utilized to identify the optimal network (Aviso et al. 2010b; Tan et al. 2011).

$$\max = \lambda \tag{13}$$

$$\lambda \in [0,1] \tag{14}$$

$$f(x,y) \leq f(x,y)^{L} + \lambda(f(x,y)^{U} - f(x,y)^{L}) \tag{15}$$

$$g(x,y) \geq g(x,y)^{U} - \lambda(g(x,y)^{U} - g(x,y)^{L}) \tag{16}$$

However, the realization of these exchange networks remains a challenge. The DEMATEL framework was thus used by Bacudio et al. (2016) to prioritize the identified barriers in the establishment of eco-industrial parks. Their results indicate that top management support is essential to the success of such initiatives.

Energy Efficient Systems

Improving the efficiency of energy systems are expected to contribute a lot towards reducing greenhouse gas emissions. More efficient energy systems can also be designed using PSE. It has been implemented in the design of polygeneration systems. These are systems which can utilize a single type of fuel to generate multiple energy products (e.g., heat, electricity, cooling). These are thus more efficient than conventional systems which operate independently of each other. Polygeneration systems are well integrated and can be modelled using an IO framework. An example of a polygeneration system which generates treated water, heat, power, and cooling is illustrated in Figure 4. It is prone to system disruptions as a result of its integrated structure. Thus, models for the optimal operational adjustment of these systems during crisis conditions have been developed using mathematical modelling (Kasivisvanathan et al. 2013) and the P-graph approach (Tan et al. 2014).

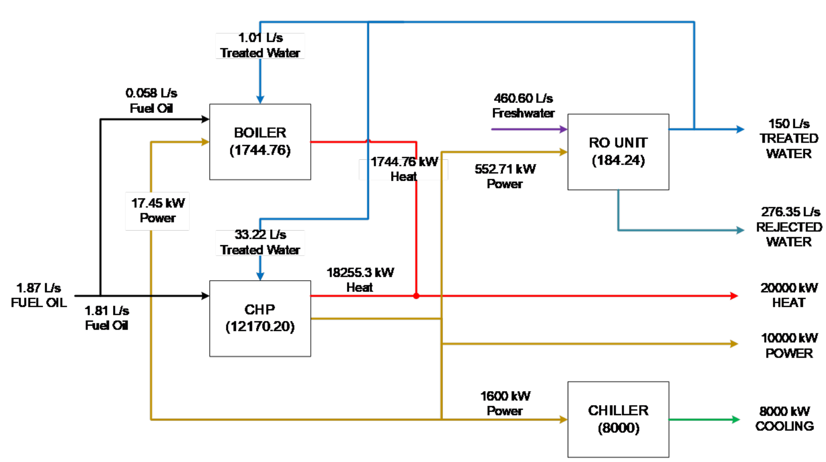

Figure 4. An example of a polygeneration system.

Such analyses are meant to provide the optimal operational condition which will minimize the disruptive effects should one process in the network fail. In addition, robust optimization models have been developed to account for any uncertainties such as price fluctuations or product demand variations, which can result in investment risks (Sy et al. 2016).

Across Product Supply Chains

PSE has also been used to identify the optimal selection of technologies for product supply chains or enterprise models. It takes into consideration multiple industries which are linked by virtue of the supply chain. Such models become useful for analyzing the impact of climate change, which manifests through the reduction in the availability of natural resources. The recent pandemic has further emphasized how the inoperability of one sector in the economy affects the performance of other economic sectors (Yu and Aviso 2020). Tan et al. (2016) developed a fuzzy optimization model to examine how resources should be adequately allocated to maximize profits and meet product demands when resources become limited in industrial complexes.

Across Economic Sectors

Economic systems can be assessed for sustainability using PSE tools. Tan et al. (2018) utilized pinch analysis to identify potential strategies which can be implemented to meet national carbon emission reduction targets amidst economic growth. It is possible to identify strategies for CO_2 reduction through the implementation of more efficient technologies across industrial sectors or increasing the proportion of renewable energy in the electricity grid. The integration of PSE and IO analysis was used by Tan et al. (2018) to identify which economic sectors should experience higher economic growth rates within the period of analysis. Results suggest that CO_2 intensive sectors should be moderated. A closer examination of these candidate strategies can be utilized to develop national policies which will encourage the growth of environmentally friendly economic sectors and control sectors which are highly pollutive.

CONCLUSION

Process systems engineering which is a computational sub-field of chemical engineering provides powerful tools for identifying the optimal design of industrial systems to make them more sustainable. Integrating PSE concepts with input-output analysis, industrial ecology, circular economy, and life cycle assessment can provide powerful insights towards the development of strategies and policies to improve industrial systems at various levels. These can be implemented for eco-industrial parks, across product supply chains, and even for the examination of regional and multi-regional economic sectors. There is much that can be explored for future work. Models can be extended to consider how new technologies can be integrated to improve system resilience. The emergence of big data analytics should also be exploited to improve assumptions on data and system performance. Furthermore, these tools can be used for the analysis of more radical solutions to the reduction of carbon emissions such as negative emission technologies.

ACKNOWLEDGMENTS

This paper is supported by the Philippine Department of Science and Technology–National Academy of Science and Technology. Furthermore, the author would like to acknowledge all collaborators who have contributed to the growth of research in the field.

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