Journal of Cleaner Production 124 (2016) 132–141

Contents lists available at ScienceDirect

Journal of Cleaner Production

journal homepage: www.elsevier.com/locate/jclepro

New composite sustainability indices for the assessment of a chemical process in the conceptual design stage: case study on hydrogenation plant

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ARTICLE INFO

Article history:
Received 31 August 2015
Received in revised form
22 February 2016
Accepted 25 February 2016
Available online 9 March 2016

Keywords:
Composite sustainability index
Energy impacts index
Safety risk index
Inherently safer design
Sustainability development
Conceptual hydrogenation process design

ABSTRACT

Sustainability indices are increasingly recognized as a powerful tool for assessing the performance of chemical process designs considering energy, environment, safety and technological improvement aspects and above all, economy. Sustainability indicators enable decision makers to simplify, quantify and analyze complex information. Generally, it is challenging to evaluate the performance of process designs on the basis of a large number of indicators. The integration of a set of key sustainability indicators in the form of a composite index is essential for simplifying the evaluation of sustainability performance. Currently available methodologies for sustainability assessment of process designs require detailed process data, which are typically unavailable at the conceptual design phase. This paper introduces a new composite sustainability index (*CSI*) that addresses the sustainability performance of chemical processes and which can be applied for early design phases where minimum amount of data are available. The three pillars of sustainability are considered in the development of the new composite index, which are energy, environmental and safety aspects. A conceptual decision model based on the analytical hierarchy process can be employed to compare and determine weights for the different sustainability indicators, which are then aggregated to obtain the *CSI*, when the indicators conflict. The capability of the proposed model is investigated by applying it to a hydrogenation case study to choose the more sustainable design among different alternatives.

1. Introduction

The path to continuous development of the products and services used by society without huge negative impact upon the Earth is called sustainability (Cobb et al., 2007).

Composite sustainability indicators are an innovative approach to evaluating the sustainability of process designs whose main feature is their effective utilization to summarize and condense dynamically complex sustainability data into manageable and simplified amount of information that can be easily analyzed (Chen and Shonnard, 2002).

Today, the concept of sustainability is widely employed in a variety of researches from molecular level (Manley et al., 2008) to teaching purposes (Carew and Mitchell, 2008) and designing sustainable products such as sustainable vehicles (van Lante and van Til, 2008). Corporations may use sustainability to integrate their following areas of concerns (Amimi and Bienstock, 2014): (a) corporate's strategy and stakeholders external communications; (b) organization's supply chain; (c) strategic decisions and design processes based on economic, eco-environmental, and equity-social concerns, to name a few.

Examples include: (a) Dow Jones Sustainability Indices (2013), which lead to high levels of skills in different areas such as strategy, financial, customer and product, governance & shareholders, and human resources; (b) FTSE4Good Environmental Leaders Europe 40 Index (2015), which delivers a tool for investors who are looking for European partnership in practical environmental management; (c) *AIChE* Sustainability Index (*SI*) based on a set of features that form a consolidated Sustainability Index or *SI* (Cobb et al., 2007). The required information is gathered from company's annual sustainability report, industrial performance rankings, government's pamphlet and newsletters. The metrics are scaled from 0 to 7 and depicted on a spider chart.

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http://dx.doi.org/10.1016/j.jclepro.2016.02.107
0959-6526/

List of abbreviations

A	Equipment size in their corresponding units (e.g. heat transfer area in m^2 for heat exchangers)
AHP	Analytical Hierarchy Process
C_P	Equipment cost ($)
f_i	Frequency of Accidents for Chemical i
H_i	Hazard Effects of Chemical i,
HV	Heating value of a fuel
$\dot{I}_e$	Rate of gas emissions to atmosphere in the form of heat or electricity consumption in a process unit
$\dot{I}^{(t)}_{gen}$	Rate of total PEIs generated or consumed by chemical reactions within the process.
$\dot{I}^{(t)}_{in}$	Rate of total potential environmental impacts existing in the input streams to the system
$\dot{I}^{(t)}_{out}$	Rate of total potential environmental impacts existing in the output streams from the system
I_{System}	Quantity of potential environmental impact inside the chemical process system
K_1, K_2 and K_3	Correlation parameters along with the minimum and maximum values of equipment size
KPI	Key Performance Indicators
M_j	Chemicals Inventory (tonne)
MW_i	Molecular weight of component i
MW_j	Molecular weight of component j
η_k	Total efficiency of a process unit k
PEI	Potential Environmental Impacts
$\dot{Q}_i$	Fraction of the heat flow attributed to component i
$(R.I)^P$	Risk Index Associated with Product Streams
$(R.I)^T$	Sum of Risk Index of Product & Waste Streams
$(R.I)^W$	Risk Index Associated with Waste Streams
US EPA	US Environmental Protection Agency
x_i	Mass fraction of component i
$x_{i,j}$	Mass Fraction of Component i in Stream j ($i, j = 1, 2, \ldots$)
WAR Algorithm	WAste Reduction Algorithm

These sustainability indices have a number of pros that escalate company's profits. However, the society approach of above mentioned sustainability indices deal with customer satisfactions and after sales services. Besides, the sustainability indices have business nature and therefore, they are based on individual company's performance and cannot be used at primary stage of a process design. The *AIChE's SI* has tried to overcome this shortcoming; however, in order to resolve this issue successfully, they need a large number of data, which vary from company to company based on business performance. Above all, none of the existing indices can be used for prototype chemical products.

Having said this constructive perspective of sustainability, Ordouei et al. (2015) have introduced new sustainability indices for product design employing environmental and energy impacts and risk reduction associated with the new products.

The implementation of quantitative energy, environmental and safety risk assessment measures in early design stages allows engineers to easily determine an adequate evaluation of the environmental burden of process design.

As the highest impact of decisions lies at conceptual design stage (Lewin, 2004), sustainable design development has become a leading goal of policy makers and researchers that takes into account environmental, societal and economic aspects, and which can be easily monitored using sustainability indicators. The use of indicators allows the translation of sustainability issues into quantifiable amounts that facilitate achieving more sustainable design of chemical processes. Several reported frameworks propose sustainability indicators that are generally measured in different units.

Process design and optimization is conducted for the establishment of new facilities, the integration of new technologies, or the retrofitting of existing processes. It typically involves standard procedures that are sequentially performed, from data gathering and process synthesis in the early design stages, to detailed design. The typical process design is based on economic objectives, such as net present value, capital investment costs, and operations and maintenance costs (Zhang et al., 2008). The environmental impacts associated with a process are typically given low priority in the design stages, and are incorporated just as end-of-pipe treatment, such as waste treatment facilities, incinerators, etc. Such design approaches overlook the environmental impacts of materials and energy used in a process plant, which causes the generation of large quantities of waste materials and pollutants (EPA, 2012). This results in significant environmental control costs to be incurred, especially with increasingly stringent environmental regulations (Chen et al., 2002). Therefore, there has been a growing interest by industries in the incorporation of more performance measures in the process design stages, such as safety, energy, environment, reliability and flexibility (Chen and Shonnard, 2002).

The procedure for the development of a sustainable design of a chemical process should incorporate the improvement of its environmental and safety performances in order to meet environmental and safety regulations, and it should be assessed using various impact categories in order to provide a more extensive evaluation of environmental effects and process hazards. The evaluation of the environmental performance of a chemical process should start from the early design stages using simplified screening procedures to more accurate assessments during detailed design (Adu et al., 2008).

Multiple production routes incorporating different configurations of various equipment can be used for the production of a certain chemical product. Screening methods can be applied in early design stages to eliminate unpromising alternatives, which plays a significant role in reaching sustainable design objectives. Attempts for improving environmental performance at later design stages holds a significantly lower potential in reducing wastes and emissions (Chen and Shonnard, 2002). Various performance evaluation methods involve the calculation of indices based on mass of pollutant emissions and waste streams, as well as toxicity-weighted mass indices for risk assessment applications.

Sugiyama et al. (2009) have investigated the role of economic and environmental assessment results to changes in the ranking of design alternatives (e.g. reaction routes, recycling configurations, operating conditions, etc.) and evaluation settings (e.g. indicator methods). Other methodologies include material balance environmental index that evaluates the environmental impact of toxicities emitted (Torres et al., 2011), and the development of a rigorous simulation model of the process in hand for which economic and environmental objectives are generated. The environmental objective is geared towards minimizing: (a) the use of natural resources and environmental impact potential (Li et al.,