Contents lists available at ScienceDirect

Chemical Engineering Research and Design

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

Multi-criteria decision analysis for the selection of sustainable chemical process routes during early design stages

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ARTICLE INFO

Article history:
Received 22 September 2015
Received in revised form 10 June 2016
Accepted 2 July 2016
Available online 11 July 2016

Keywords:
Sustainability
Sustainability indicator
Sustainable process design
Chemical process route selection
Multi-criteria decision analysis
Sustainable Cumulative Index

ABSTRACT

Decision-making for sustainable design requires the evaluation of different options considering all sustainability dimensions simultaneously: economic, environmental and social. Each dimension has a specific relative importance, which depends on the process that is being assessed. The determination of the relative importance is not a simple task, principally, during early design stages when detailed information about the process is scarce, and when core decisions affecting the entire design are made. An example of this kind of decisions during early design stages is the selection of the chemical process route, which, once defined, provides the guidelines for the process design. The present study proposes a multi-criteria analysis based methodology to evaluate different chemical process route options under sustainability criteria and to guide the selection among them. The methodology uses normalized indicators to assess each sustainability dimension, and a multi-criteria analysis method (MCDA) to calculate the weights and influences between dimensions. Indicators, dimension weights and influences are integrated into the Sustainable Cumulative Index (SCI) that can be used to compare chemical process route options in sustainability terms and to support their selection. The proposed methodology is illustrated through the assessment and selection of a chemical process route to produce ethyl acetate.

1. Introduction

Currently, the application of sustainability principles in the chemical industry is a general concern. This is increasingly reflected in legal regulations and industrial practices, as well as in education and scientific fields. For example in Europe since 2007, the REACH regulation (Registration, Evaluation, Authorization and Restriction of Chemicals) places the responsibility on industries to manage risks from chemicals and to provide safety information on such substances (EC Environment, 2015). Similarly, the United States Environmental Protection Agency (EPA) is working to examine the scope of the chemicals included in the Toxics Release Inventory (TRI) program, providing communities with more information on the issue (EPA, 2015). Non-governmental institutions such as the International Organization for Standardization (ISO) have been supporting this trend by establishing requirements for environmental management in the ISO 14000 standard and for social

Abbreviations: SCI, Sustainable Cumulative Index; MCDA, multi-criteria analysis method; IWF, integrated weighting factor; AHP, Analytic Hierarchy Process; DEMATEL, Decision-Making Trial and Evaluation Laboratory.

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http://dx.doi.org/10.1016/j.cherd.2016.07.001

responsibility in the ISO 26000. In the same direction, an increasing number of higher education institutions have incorporated the principles of sustainable development into their curricula, as analyzed by Lozano (2010, 2003).

Even if awareness of developing sustainable chemical processes has been a hot topic for some years, the industrial sector is still in search of practical tools to conduct systematic sustainability assessments of existing processing technologies as well as new ones (Othman et al., 2010). In general, the design task requires assessing different alternatives in order to decide which of the options constitutes the best choice according to an objective function (traditionally process economics). It is desirable that the decision-making process becomes rational and structured rather than intuitive or subjective. This can be difficult when analyzing chemical processes from an integrated sustainability approach, because it requires the simultaneous consideration of the economic, environmental, and social dimensions. This can be more demanding during early design stages, because the conceptual process is not defined and the main process variables are unknown. In this context, appropriate assessment methods for each dimension and tools to make decisions involving multiple conflictive objectives are needed.

There are several studies and methodologies that can be used to evaluate process design options in terms of sustainability. They differ in the assessment method used, the completeness (partial or integral sustainability), and the design stage in which they can be applied. Most methods can only be implemented during advanced design stages, when enough information is available to perform the material and energy balances for the entire process. Examples of these methods are life cycle assessment (LCA) for environmental impacts (Azapagic, 1999), quantitative risk assessment (QRA) for risk estimation (Arendt, 1990; Papazoglou et al., 2003), and the widely used qualitative methods such as failure mode and effects analysis (FMEA) and hazard and operability study (HAZOP) for reliability and safety analysis.

However, in order to obtain sustainable products, processes and plants, actions must be taken at the very early stages of the design process when the most important decisions are made (Banimostafa et al., 2012). During these stages, after product properties are established, possible chemical process routes are searched and screened, and only the most promising ones are further analyzed. The term chemical process route is used here according to the definition given by Edwards and Lawrence (1993): the raw material(s) and the sequence of chemical reaction steps that convert them to the desired product(s). A chemical process route can have more than one chemical reaction. According to Hassim and Edwards (2006) and Srinivasan and Nhan (2008), the choice of a chemical process route is one of the key decisions in early design stages. Its selection defines possible raw materials to be used in the process and their pretreatment (upstream operations), as well as reaction conditions (phase, type of catalyst, etc.), and it also constrains the design of the downstream operation. In this sense, it is important to avoid negative effects on sustainability dimensions by their systematic consideration from the beginning of the design process.

Several authors have suggested different sustainability indicators to measure the performance of alternatives in early design stages. Carvalho et al. (2008) presented a methodology to calculate the economic performance during the chemical process route selection. Their methodology, besides performing the cash flow analysis between input costs and revenues from product sales, considers side reactions, byproducts and energy costs. Similarly, some approaches have been proposed to measure the environmental impact of chemical process routes, which include, among others, the Environmental Hazard Index (EHI) proposed by Cave and Edwards (1997), the Waste Reduction algorithm (WAR) proposed by Young et al. (2000) and the environmental potential impact (EPI) proposed by Li et al. (2009). The social dimension can be quantitatively represented at the early design stage through safety and health indicators. Safety has been extensively studied because workers' lives depend on the establishment of safe conditions in chemical processing plants. Right decisions during early design stages can reduce or remove risks, which is called inherent safety design. Inherent safety assessment methods include the Inherent Safety Index (ISI and ISI2) referenced by Adu et al. (2008) and the Prototype Inherent Safety Index (PIIS) proposed by Edwards and Lawrence as reviewed by Rahman et al. (2005). Some approaches have been presented for occupational health indicators, which are perhaps less studied than any others, including the Process Route Healthiness Index (PRHI), the Inherent Occupational Health Index (Hassim and Edwards, 2006) and the graphical method to evaluate the inherent occupational health hazards (Hassim et al., 2013).

Two aspects have to be covered in order to apply indicators toward the calculation of an integrated sustainability assessment. First, it is necessary to standardize the indicators that describe each dimension, because they have different meanings, definitions and units. Second, the information given by all indicators has to be presented simultaneously so that decision-makers can visualize eventual trade-offs between alternatives and identify the best in terms of sustainability.

An interesting approach for accomplishing the first aspect was proposed by Srinivasan and Nhan (2008). They classified the indicators into those that are defined in an interval or ratio scale and are easy to normalize, and those that are not. For the latter they proposed normalization based on frequency distribution for common reactions, avoiding subjective scaling.

Concerning the second aspect, common approaches are the addition of normalized indicators without weighting (Srinivasan and Nhan, 2008), weighting them according to industrial practices (Sugiyama et al., 2006; Albrecht et al., 2010; Banimostafa et al., 2012) or weighting them in relation to local management policies (Tugnoli et al., 2008). Other approaches integrate the sustainability indicators using graphical representations or statistical techniques. Some authors proposed tools such as principal component analysis (PCA) (Sugiyama et al., 2006), sensitivity analysis and graphical multi-objective evaluation (Banimostafa et al., 2012). These methods allow process designers to identify key indicators, visualize trade-offs and provide information on the mutual dependence of different criteria, but are merely descriptive.

Another alternative to integrate the sustainability indices is the implementation of multi-criteria decision analysis (MCDA), which is addressed in the present study. The use of MCDA to solve sustainability problems was carried out by Othman et al. (2010), using Analytic Hierarchy Process (AHP) to support decision-making during chemical process design. It was also used by Santoyo-Castelazo and Azapagic (2014), who implemented MCDA for a sustainability assessment of energy systems. More cases where MCDA methods were applied to chemical engineering problems are listed in Table 1.

The choice of a particular MCDA method is strongly linked to the characteristics of the problem, the nature of available data, and the main goal. For the application of a specific MCDA method during early design stages, it should be considered that the relative importance of the sustainability dimensions could change from one chemical industry to another, and that there is a mutual relation among the different sustainability dimensions. In this regard, the present study proposes a methodology for chemical process route selection during early design stages that address these two aspects: the relative importance through the integration of the Analytic Hierarchy Process (AHP) and the interrelation between the dimensions by the Decision-Making Trial and Evaluation Laboratory (DEMATEL) (Chou et al., 2012; Abdullah and Zulkifli, 2015; Chou et al., 2010). The proposed methodology calculates an integrated sustainability index called Sustainable Cumulative Index (SCI) on the basis of normalized sustainability indicators using MCDA methods. Indicators assess the performance of alternatives in each dimension, while MCDA methods integrate assessments according to the specific characteristics of the process to be designed. The application of MCDA methods is normally based on the opinion of experts or in data analysis. In this case, we used the opinion of experts to formalize the technical knowledge that helps to define the importance and interrelation of criteria.

To illustrate this methodology, it was applied for the selection of the most sustainable chemical process route to produce ethyl acetate among four different alternatives. The integrated AHP-DEMATEL method was applied based on the opinion of two groups of decision-makers: experts from industry and academia and undergraduate students of chemical engineering. Although the methodology shown in this article was implemented in the selection of a chemical