Biochemical Engineering Journal 116 (2016) 146–156

Contents lists available at ScienceDirect

Biochemical Engineering Journal

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

Regular article

A framework for techno-economic & environmental sustainability analysis by risk assessment for conceptual process evaluation

Carina L. Gargalo [a], Ana Carvalho [b], Krist V. Gernaey [a], Gürkan Sin [a,*]

[a] CAPEC-PROCESS Research Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark
[b] CEG-IST, Instituto Superior Técnico, Universidade de Lisboa, Portugal

ARTICLE INFO

Article history:
Received 27 January 2016
Received in revised form 22 May 2016
Accepted 6 June 2016
Available online 7 June 2016

Keywords:
Conceptual process
Techno-economic assessment
Environmental assessment
Uncertainty analysis
Glycerol biorefinery

ABSTRACT

The need to achieve a sustainable process performance has become increasingly important in order to keep a competitive advantage in the global markets. Development of comprehensive and systematic methods to accomplish this goal is the subject of this work. To this end, a multi-level framework for techno-economic and environmental sustainability analysis through risk assessment is proposed for the early-stage design and screening of conceptual process alternatives. The alternatives within the design space are analyzed following the framework's work-flow, which targets the following: (i) quantify the economic risk; (ii) perform the monetary valuation of environmental impact categories under uncertainty; (iii) quantify the potential environmental risk; (iv) measure the alternatives' eco-efficiency identifying possible trade-offs; and, lastly (v) propose a joint risk assessment matrix for the quantitative and qualitative assessment of sustainability at the decision-support level. Through the application of appropriate methods in a hierarchical manner, this tool leads to the identification of the potentially best and more sustainable solutions. Furthermore, the application of the framework is highlighted by screening two conceptual glycerol bioconversion routes to value-added chemicals namely 1,3-propanediol (1,3-PDO) and succinic acid.

1. Introduction

Global concerns about climate change, energy security, exhaustion of fossil resources and its societal impacts, have become important for policy and decision-makers. These facts lead to new challenges for the (bio)chemical and processing industries, which motivate researchers to incorporate sustainability matters into the design of new chemical and biochemical processes. Therefore, the bio-based economy has been seen as a key approach that may meaningfully lead to long term sustainable development, where bio-based chemicals and fuels may play a relevant role that will potentially contribute to the replacement of oil-based resources [1]. Due to the multidimensional nature of sustainability, the design and analysis of sustainable biorefineries is built on multi-criteria and multi-objective decision making procedures, leading to complex problems. The complexities arise not only from the multi-evaluation techniques to be chosen, but also from the significant amount of input data required to perform the sustainability analysis, data which may originate from different sources, with different degrees of uncertainty [2,3]. The comparison and screening of potential processes at the conceptual design phase of biorefineries is marked by assumptions, hypotheses and simplifications that need to be made in order to represent the complexity of the problem. Therefore, it implies that during the first stages of biorefinery design and development, since real data is often incomplete or not available, there are several alternative technologies, feedstocks and products, generating a great number of potential processing pathways. Hence, there is a need for screening and gathering the most appropriate processing networks regarding economics, environmental constraints and overall sustainability. Consequently, uncertainty on the techno-economic parameters/criteria is expected, and needs to be appropriately dealt with [4].

Furthermore, uncertainty in environmental assessment originates from, among others, inaccurate measurements, lack of data and erroneous model assumptions (inaccurate or unreliable assumptions when the modeler has to make decisions under limited or no data availability) [5]. For the sake of simplicity, data uncertainty is divided into lack of data (data gaps or lack of representative data for the studied system) and data inaccuracy [6].

There are several proposed approaches on how to deal with error propagation, such as, fuzzy logic [7], Gaussian formulas [8,9] and

* Corresponding author.
E-mail address: gsi@kt.dtu.dk (G. Sin).

http://dx.doi.org/10.1016/j.bej.2016.06.007
1369-703X/

the Monte Carlo technique, as the most commonly used methods for propagation of parameter uncertainty [10–14].

Despite the considerable work being done on the development of initiatives to include propagation of uncertainty in environmental assessments [10,15], the results are usually reported based on deterministic data [10,16].

Regarding deterministic models, a good decision is based on the outcome on its own. However, in very few decision-making circumstances, perfect/complete information is available for the decision maker (i.e. all the needed data with sufficient accuracy is present). The majority of decisions are made in spite of uncertainty, where probability comes into the process as a representation of complete knowledge [17]. Hence, probability assessment stands out as quantification of uncertainty and as an important tool for both communicating uncertainty and managing it.

Furthermore, under uncertainty conditions, the decision maker is concerned not only with the value of the outcome but also with the extent of risk that each decision carries. Quantified based on the uncertainty for which the probability distribution is known (or projected), risk is equal to the sum of probabilities of outcome(s) (likelihood of occurrence) times the projected loss as a consequence of the outcome(s).

Consequently, risk-based decision-making provides information in an organized structure about the possibility of one or more unwanted outcomes to occur and its potential economic loss. This information helps managers towards more informed and realistic choices regarding project feasibility.

Examples of studies/methodologies used to compare alternatives based on predefined criteria/indicators and their integration are: Azapagic et al. [18], where a methodology is presented to guide the user through different design stages for the integration of technical, economic, environmental and social criteria; Sacramento-Rivero [19] proposes a performance assessment methodology applicable to biorefineries where a sustainability scale is used based on an absolute reference, and normalized for sustainability indicators applicable to biorefineries; Martinez-Hernandez et al. [20] introduce a tool that result from the combination of the value analysis method for the evaluation of economic potential with environmental footprinting for impact analysis; Sacramento-Rivero et al. [21] illustrate the integration of sustainability indicators for the design of a potentially sustainable switchgrass biorefinery; and, Sanchez et al. [22,23] use a framework that aims at the calculation of the overall impacts, for both economic and environmental domains and provide information that could be used to improve the sustainability of the processes under analysis.

Another approach is to identify the optimal solution among different alternatives based on a given objective function. Authors in [24–26] present a literature review on programming techniques explored to identify the optimal alternative through single or multi-objective optimization.

Notwithstanding that many studies focused on the economic and environmental domains of sustainability, it should be noted that the majority of these studies measure sustainable performance solely under deterministic conditions, where uncertainty and the associated risk a decision carries, is disregarded. Accordingly, as far as we are aware, no other studies have proposed a combined techno-economic and environmental risk quantification matrix for sustainability assessment and decision-making. Therefore, this work proposes a step-by-step framework whose purpose is to identify the best potential alternative(s) that would sustainably create value with the least potential risk of economic and environmental impact. This is achieved by systematically integrating uncertainty and sustainability analysis into a risk assessment framework. The framework aims to stablish a holistic view regarding the following: (i) estimation of the deterministic economic and environmental metrics; (ii) use of Monte Carlo technique for propagation of uncertainties to the environmental and economic indicators; (iii) quantification of the economic risk; (iv) monetary valuation of environmental impact categories under uncertainty; (v) quantification of the potential environmental risk; (vi) use of the sustainability risk matrix as a visual tool for quantitative and qualitative analysis for decision-making. Moreover, performing qualitative analysis by making use of the sustainability risk assessment matrix (as a visual aid tool), is a valuable advantage/benefit of the framework which facilitates exchange of information among experts and non-experts.

The remaining sections of this article are structured as follows: (i) the framework section introduces a step-by-step explanation (user guide) of how to use the quantification of risk as an integrating tool decision-making; then (ii) the framework is highlighted through its application to a relevant case study, the glycerol valorization to value added products namely 1,3-PDO and succinic acid; and finally, (iii) conclusions from the work are presented.

2. Decision-support framework for techno-economic & environmental sustainability analysis by risk assessment for conceptual process evaluation

The proposed framework is based on the combination of two previously presented methodologies, where a methodology for environmental assessment under uncertainty was proposed [27] and an algorithm for the techno-economic assessment under uncertainty was presented [28]. These two methodologies are now combined, and the analysis is taken a step further by incorporating a quantitative and qualitative sustainability analysis by risk assessment. Therefore, the framework's main goal is to systematically, at an early stage of process design, collect, evaluate and screen the alternatives within the design space, through a comprehensive sustainability analysis by risk assessment.

As presented in Fig. 1, the framework work-flow is composed of six steps: (1) problem definition; (2) data collection and management; (3A) deterministic techno-economic analysis; (3B) deterministic environmental analysis; (4) Monte Carlo technique for uncertainty analysis; (5) economic and environmental risk quantification; and, (6) risk assessment and decision-making.

2.1. Step 1: problem definition

In this step, as shown in Fig. 1, the user (decision-maker) has to define if the problem is to be solved through a process- or product-oriented approach.

A product-oriented approach is recommended when, the aim is to produce a specific product (or a set of products) and the decision-maker wants to evaluate several paths for its production. This is the case of a retrofit problem, where one wants to change or adapt the existing plant in order to have more production routes and/or to have different sources of feedstock being converted in the plant. Whereas a process-oriented approach should be used when the user is aiming to evaluate a number of paths to synthetize a set of products from a certain (already selected) raw material and, therefore, the question is the selection of product portfolio. Then it would result in a completely new plant. Based on this, the system boundaries and the functional unit (FU) should be defined. Hence, the framework application would assist the decision-maker to systematically draw the analysis boundaries and define the functional unit (FU).

2.2. Step 2: data collection & management

The Step 2, as shown in Fig. 1, targets to establish the design space from which the potential best alternative will be identified.