Computers and Chemical Engineering 82 (2015) 362–373

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Optimal processing pathway selection for microalgae-based biorefinery under uncertainty

Muhammad Rizwan[a], Muhammad Zaman[a], Jay H. Lee[a,*], Rafiqul Gani[b]

[a] Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 305-701, Republic of Korea
[b] CAPEC, Department of Chemical & Biochemical Engineering, Technical University of Denmark, 2800 Kgs Lyngby, Denmark

ARTICLE INFO

Article history:
Received 15 June 2015
Received in revised form 3 August 2015
Accepted 4 August 2015
Available online 12 August 2015

Keywords:
Biofuels
Microalgal biorefinery
Uncertainty analysis
Stochastic mixed integer nonlinear programming (sMINLP)
Decision-making under uncertainty

ABSTRACT

We propose a systematic framework for the selection of optimal processing pathways for a microalgae-based biorefinery under techno-economic uncertainty. The proposed framework promotes robust decision making by taking into account the uncertainties that arise due to inconsistencies among and shortage in the available technical information. A stochastic mixed integer nonlinear programming (sMINLP) problem is formulated for determining the optimal biorefinery configurations based on a superstructure model where parameter uncertainties are modeled and included as sampled scenarios. The solution to the sMINLP problem determines the processing technologies, material flows, and product portfolio that are optimal with respect to all the sampled scenarios. The developed framework is implemented and tested on a specific case study. The optimal processing pathways selected with and without the accounting of uncertainty are compared with respect to different objectives.

1. Introduction

Under the broad concept of microalgal biorefinery, microalgae is to be cultivated and processed to produce a wide range of products such as biofuels, chemicals, animal feed, pigments, power/heat, etc. (Yen et al., 2013; Rawat et al., 2013). Despite the various claimed benefits associated with the development of microalgae based biorefinery (such as potentially significant improvements in the overall economics of biofuels), there are many challenges yet to be overcome. These challenges include (1) existence of a large number of potential processing pathways for the biorefinery development, and (2) inconsistency and shortage in the process information available in the literature because the involved processing technologies are still at a nascent stage. Potential development of additional technologies as well as the likely future improvements further increases the uncertainty one faces at the current preliminary assessment phase. Consequently, the optimal biorefinery configuration determined based on uncertain parameters can prove to be highly suboptimal later due to discrepancies among the assumed and actually realized parameter values. Therefore, it becomes necessary to identify the optimal biorefiney configurations with due considerations given to the effect of the existing uncertainties in order to ensure robust decision making.

Process systems engineering's tools and concepts can be applied to address these challenges of microalgal biorefinery by developing a systematic modeling framework to determine the optimal biorefiney configurations in a cost effective, robust, and environmentally sustainable manner (Liu et al., 2009; Yue et al., 2014). Under the domain of energy systems engineering, stochastic programming/optimization is a widely used tool to determine the optimal processing networks under stochastic uncertainty, and this approach has been presented in many studies (for example, Dua and Pistikopoulos, 1998; Grossmann, 2005). Karuppiah and Grossmann (2008) proposed a two stage stochastic model to determine the optimal design of an integrated water system under uncertainty. A superstructure was optimized under uncertainty that incorporates all feasible design alternatives for wastewater treatment, reuse, and recycle. Kim et al. (2011) addressed the challenge of stochastic uncertainty for the optimal design of biomass supply chain networks by formulating a two stage stochastic mixed integer program. The robustness and global sensitivity of stochastic design vs. nominal design was analyzed via Monte Carlo simulation. Quaglia et al. (2013) developed a systematic framework for enterprise-wide optimization in order to determine the optimal process networks under uncertainty. The developed framework was implemented on an industrial case study where a stochastic mixed-integer nonlinear programming (sMINLP) model was

* Corresponding author. Tel.: +82 42 350 3926; fax: +82 42 350 3910.
E-mail address: jayhlee@kaist.ac.kr (J.H. Lee).

http://dx.doi.org/10.1016/j.compchemeng.2015.08.002
0098-1354/

formulated and solved to identify optimal processing of soybean oil under uncertainty. Cheali et al. (2014) adapted this framework for the purpose of determining optimal processing networks under uncertainty for lignocellulosic biorefinery. The impact of market price uncertainties on the optimal solution was evaluated by integrating superstructure based process synthesis approach with uncertainty analysis.

The effect of uncertainty on the optimal configurations of microalgae-based biorefinery has not been evaluated yet. However, many studies on microalgae-based biorefinery have been carried out recently but all these contributions focus only on identifying optimal processing networks for the production of biofuels from microalgae under a deterministic model (Rizwan et al., 2013a, 2013b, 2015; Gebreslassie et al., 2013; Gong and You, 2014a, 2014b). It is thus the objective of this paper to address and evaluate the effect of uncertainty on the optimal processing pathway for a microalgal biorefinery.

In this paper, a framework to determine the optimal/promising processing pathways for the production of biofuels from microalgae by considering the effect of uncertainties present in microalgal biorefinery design is proposed. The proposed framework is based on biorefinery superstructure model developed in an earlier study (Rizwan et al., 2015), which has been extended to handle and address the uncertainties in the problem dataset so that the decisions made are robust with respect to them. First, a sensitivity analysis is performed to select the influential key parameters for the uncertainty analysis so as to reduce the design problem to a manageable size. The problem of determining the optimal biorefinery configurations under given parameter uncertainties (modeled as sampled scenarios) is then formulated as a sMINLP problem and solved in the software package GAMS using a database built in Excel. The performance of the stochastic optimal solution (in terms of the average gross operating margin (GOM) over the whole set of sampled scenarios) are then computed and compared against those of the deterministic optimal solution and the "worst-case" optimal solution. The results from these optimizations and their comparison give useful technical insights about the optimal configurations of microalgal biorefinery from the perspective of both cost-effectiveness and robustness with respect to uncertainty.

2. Modeling framework

The problem of determining the optimal biorefinery configurations for the production of biofuels from microalgae by developing a superstructure based optimization model was addressed in a previous work (Rizwan et al., 2015). In this contribution, the major uncertainties have been incorporated into the biorefinery superstructure model, which leads to the formulation of a stochastic optimization model. The steps involved are described in details in this section.

2.1. Problem definition

In the first step, the problem scope is defined by identifying and selecting the objective function to be optimized with respect to various techno-economic constraints while considering the uncertainties in the important, sensitive model parameters. A general problem statement is given below.

Given is a superstructure of microalgae-based biorefinery (Fig. 1) which encompasses all the available potential technological alternatives/options for the various processing steps involved in the microalgal biorefinery, such as the cultivation of microalgae, harvesting of microalgal biomass, pre-treatment step including drying and cell disruption of harvested biomass, lipid extraction, transesterification, post-transesterification purification, pre-treatment of microalgae residue, and conversion of residue to useful products. The optimization problem is defined as to determine the optimal processing network(s) for the production of biofuels from microalgae. When the uncertainties are expressed as distributions in the parameter space or discrete scenarios sampled from it, it leads to the formulation of a sMINLP problem. The objective function chosen in this work is to maximize the expected value of GOM over the space all probable scenarios. Maximization of the average GOM over those scenarios leading to the lowest GOM values (the "worst-case" scenarios) is also examined.

2.2. Data collection and superstructure development

A biorefinery superstructure has been developed for the production of biodiesel from the lipid contents of microalgae and the simultaneous conversion of microalgae residue into the useful products, e.g., biooil, bioethanol, biogas, etc. It includes all the major known processing steps/stages for the production of biofuels from *Chlorella vulgaris*, and at each processing step various potential technological alternatives/options are considered. As shown in Fig. 1, each option included in the superstructure is represented by two indices; the first index represents the option number and the second index represents the processing stage. The list of technological options included in the biorefinery superstructure model is given in Table 1. The empty boxes represent the bypassing of certain processing stages, e.g., to accommodate wet lipid extraction, in situ transesterification, etc. The detailed description of the problem data, superstructure development and process description can be found in our previous study (Rizwan et al., 2015).

2.3. Deterministic formulation

In this step, a deterministic optimization problem is formulated and solved to find the optimal processing network with nominal parameter values while disregarding the uncertainties in them. The deterministic problem results in the formulation of a MINLP model. The detailed information on formulating MINLP model can be found in Rizwan et al. (2015). The results obtained in this step locate the deterministic optimal processing pathway for the production of biofuels from microalgae.

2.4. Selection of influential parameters/uncertain parameters

In this step, sensitivity analysis is performed based on the deterministic MINLP model (formulated in step 2.3) to investigate the effect of the 25 key model parameters (listed in Fig. 2) on the optimal solution as well as on GOM. The objective of this analysis is to identify a set of dominant parameters among the 25 parameters.

This analysis is done by varying each parameter individually, and then examining its effect on GOM (Fig. 2). The value of GOM obtained under the deterministic formulation (step 2.3) is used as a reference. Out of the 25 parameters, 11 parameters affect GOM while the rest of the parameters have no effect. Furthermore, out of these 11 parameters, 7 parameters (fractional conversion of residue into biogas, fractional conversion of residue into bioethanol, fractional conversion of lipids into biodiesel via base catalyzed transesterification, fractional conversion of lipids into biodiesel via acidic in situ transesterification, CO_2 conversion for the open pond system, CO_2 conversion for the photobioreactor, and lipid yield for the wet extraction method) affect both optimal design and its GOM value, whereas the other 4 parameters (lipid content, cost of CO_2, cost of nitrogen, and cost of phosphorus) affect the GOM only in a minor way. This analysis, thus, reveals that uncertainties in these parameters can have significant impact