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A mathematical programming formulation for biorefineries technology selection

Nikolaos Bonatsos[a], Endrit Dheskali[a], Denise M.G. Freire[b], Aline Machado de Castro[c], Apostolis A. Koutinas[d], Ioannis K. Kookos[a,*]

[a] Department of Chemical Engineering, University of Patras, Rio, 26504 Patras, Greece
[b] Department of Biochemistry, Chemistry Institute, Federal University of Rio de Janeiro, Cidade Universitária, Centro de Tecnologia, Bloco A, Lab 549, Rio de Janeiro, 21941-909 RJ, Brazil
[c] Biotechnology Division, Research and Development Center, PETROBRAS, Av. Horácio Macedo, 950. Ilha do Fundão, Rio de Janeiro 21941-915, Brazil
[d] Department of Food Science and Human Nutrition, Agricultural University of Athens, Iera Odos 75, 118 55 Athens, Greece

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ABSTRACT

Systematic methods, such as mathematical programming methods, are traditionally used in decision making concerning capacity planning, especially at tactical and operational level. However, such methods might have the greatest impact at the strategic level where substantial resources are irreversibly allocated. This study proposes a mathematical programming methodology to assist decision makers in strategic (long term) planning for bioprocessing of renewable resources. The novelty lies on the incorporation of significant detail of the bioprocess design in the strategic model and the use of a relatively accurate model for estimating the cost of manufacture of the alternative bioprocesses. A case study demonstrates the advantages of the proposed systematic methodology focusing on optimal screening of 25 bioprocesses for the conversion of molasses, sucrose and glycerol into 11 metabolic products. The methodology was validated via preliminary techno-economic evaluation of the optimum technology-mix involving the production of succinic acid, poly(3-hydroxybutyrate) and 2,3-butanediol.

1. Introduction

Conventional industrial sectors produce significant quantities of waste and by-product streams that constitute renewable resources for the development of integrated biorefineries producing bio-based chemicals and polymers as well as bioenergy. White biotechnology [1] will play a pivotal role towards the creation of numerous possibilities connecting the utilisation of renewable resources with the production of existing or novel bio-based products. According to the United States Department of Energy, “a biorefinery is a facility that integrates biomass conversion processes and equipment to produce fuels, power, and chemicals from biomass. The biorefinery concept is analogous to today’s petroleum refineries, which produce multiple fuels and products from petroleum.” [2]. The goal within the biorefinery concept is to start with a renewable feedstock-mix that will be processed by a technology-mix in order to produce a multiplicity of products in a systematic, technologically feasible and sustainable manner [3]. A prerequisite for selecting the renewable feedstock-mix is the low logistics burden associated with the production and availability of different feedstocks at a cost-competitive distance from the location of the refining facility. This is the reason why the exploitation of existing waste and by-product streams in conventional industrial facilities constitutes an attractive scenario as it does not involve significant logistics burdens.

The rate at which knowledge is generated about potential microbial bioconversions is overwhelming [4–6]. Any industrial by-product stream that is produced in significant quantities is now considered as a valuable resource rather than a waste stream. These resources are evaluated as fermentation feedstocks for the production of various intracellular or extracellular products, such as platform chemicals (i.e. selected C2–C6 metabolic products), single cell oil and bio-based polymers [5–7]. Enzymes and microorganisms are used for the production of end-products or intermediate chemicals that are used in various industrial sectors [6–8]. The possibilities have been expanded by technological advances in the utilisation of metabolically engineered microorganisms that over-produce industrially useful chemicals. The aim is to improve overall conversion, eliminate secondary products, reduce costs and finally create an efficient and sustainable route for by-product utilization.

* Corresponding author.
E-mail address: i.kookos@chemeng.upatras.gr (I.K. Kookos).

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Nomenclature

c_{el}	Is the cost of electricity ($ kWh^{-1})
c_s	Is the cost of steam ($ t^{-1})
COL	Is the cost of operating labour ($ y^{-1})
COM	Is the cost of manufacture ($ y^{-1})
CRM	Is the cost of additional raw materials such as nutrient and supplements ($ t^{-1})
CUT	Is the cost of utilities ($ y^{-1})
c_p	Is the selling price of product p ($ t^{-1}) times
c_r	Is price of raw material r ($ t^{-1})
$C_{t,p}$	Is the final concentration (titer) of product p in the fermentation broth when technology t is used (in $t\,m^{-3}$)
EP	Economic potential ($ y^{-1})
FCI	Is the fixed capital investment ($)
FCI_V	Is the fixed capital investment per unit of installed fermentation volume (k$/$m^3$ or $/L)
F_p	Mass flowarte of product p ($t\,y^{-1}$)
F_r	Mass flowarte of raw material r ($t\,y^{-1}$)
$f_{r,t}$	Is defined as the amount of raw material r that is fed to technology t ($t\,y^{-1}$)
$f_{t,p}$	Is defined as the amount of product p produced by technology t ($t\,y^{-1}$)
$N_{b,t}$	Number of batches per year
$N_{f,t}$	Number of bioreactors used in technology t
p	Set of potential products, 1,2,. . ., n_p
$p_{el,aer,t}$	Is the power consumption for aeration of fermentation broth when an aeration rate of 1 vvm is used ($kWh\,m^{-3}$)
$p_{el,agit,t}$	Is the power consumption for agitation of the bioreactor broth ($kWh\,m^{-3}$)
p_{strl}	Is the steam consumption for sterilization of the fermentation broth ($t\,m^{-3}$)
r	Set of raw materials, 1,2,. . ., n_r
t	Set of biotransformation technologies, 1,2,. . ., n_t
t_y	Is the operating hours per year (h)
$UCRM_t$	Is the cost of nutrient supplements per unit volume of the bioreactor broth ($ m^{-3})
$V_{b,t}$	the necessary total fermentation broth volume for technology t ($m^3\,y^{-1}$)
$V_{F,t}$	Total installed bioreactor volume used in technology t (m^3)
$V_{f,t}$	Volume of each bioreactor used in technology t (m^3)
vvm_t	Is the aeration rate used during the fermentation (in vvm)
$Y_{r,t,p}$	Is the yield coefficient that denotes the amount of product p produced when raw material r is used in technology t (in t of product per t of raw material)
Δ_t	Are binary variables introduced to denote adoption ($\Delta_t = 1$) or rejection ($\Delta_t = 0$) of technology t
θ	Is a constant for the calculation of the turnaround time
λ	Is the ratio of the active to total bioreactor volume (assumed as $\lambda = 0.8$)
τf_t	Is the time necessary to achieve the final concentration $C_{t,p}$ in technology t (in h)

However, the economic forces that attract capital investment for the industrial implementation of an innovative process are not the only forces applied during the diffusion of novel technologies into the economy [9,10]. This explains partially the slow rate at which white biotechnology is adopted by the industry. Technical and economic feasibility are necessary (but not sufficient) conditions to turn any invention into industrial practice. Basic and sound engineering facilitates the process of transforming an invention into innovation. Given the plethora of available biotransformations the aim is to develop engineering tools so as to evaluate their technical and economic characteristics with sufficient accuracy in acceptable time scales. This excludes exhaustive enumeration and evaluation of all available routes. This is by no means a recent challenge [10–12]. The problem of technology selection is among the most important, most difficult and most well-studied problems in systems engineering. Technology selection is part of the long term, strategic capacity planning problem.

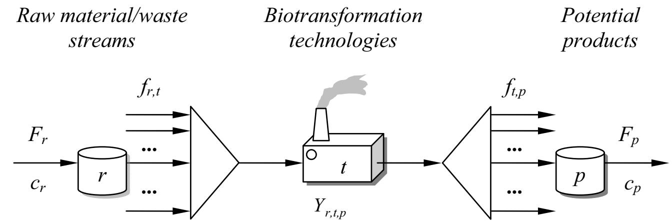

Fig. 1. Simplified representation of the superstructure used in the mathematical model.

Quantitative methods, such as mathematical programming methods, are traditionally used in decision making concerning capacity planning, especially at tactical and operational levels [13–15]. However, it is the strategic level at which the use of quantitative methods might have the greater impact as decisions at this level allocate irreversibly substantial resources. The reasons that make the incorporation of mathematical programming methods in the strategic planning of bioprocesses difficult are the complexities of the underlying bioprocess, the uncertainty of market demand for the potential products and the high degree of market flexibility required regarding both raw materials and end-products (e.g. numerous raw materials can be used to produce the same target molecule and numerous target molecules can be used to satisfy the same industrial or market need) [10,12].

The aim of this work is to propose a mathematical programming methodology that can be used in assisting decision makers to undertake decisions related to the strategic (long term) planning of the valorization of renewable resources via white biotechnology. The novelty of the work presented is that it incorporates significant details of the bioprocess design at the strategic model and also use is made of a relatively accurate model for estimating the cost of manufacture of the alternative bioprocesses. The selection of the most promising technologies for valorization of renewable resources within the biorefinery framework is therefore based on a relatively accurate economic model that allows the efficient evaluation and ranking of alternatives. Complete enumeration and detailed evaluation of alternative bioprocesses is thus avoided and promising solutions can be isolated quickly. A case study is carried out to prove this concept. The renewable resources selected were sucrose, sugarcane molasses and glycerol. The selection of 11 metabolic products and 25 alternative bioprocesses leading to the production of the metabolic products was based on publications available in the open literature. The proposed systematic mathematical programming methodology is validated via techno-economic evaluation of the most promising technology-mix scenario.

2. Proposed methodology and mathematical formulation

2.1. Basic elements of the proposed mathematical formulation

The system considered in this study is presented in Fig. 1. It is assumed that $r = 1, 2,\ldots,n_r$ raw materials are available for potential valorization at a maximum quantity of F_r (in $t\,y^{-1}$). These raw