Bioresource Technology xxx (2013) xxx–xxx

Contents lists available at ScienceDirect

Bioresource Technology

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

Development and validation of a technoeconomic analysis tool for early-stage evaluation of bio-based chemical production processes

Joshua T. Claypool, D. Raj Raman *

Agricultural and Biosystems Engineering Department, 3222 NSRIC, Iowa State University, Ames, IA 50010-3310, United States

HIGHLIGHTS

- Multi-stage bioprocesses that convert sugar to chemicals are of commercial interest.
- We model these processes by making simplifying assumptions.
- Our model estimates the cost of producing a chemical through a specific route.
- Early-stage cost estimates are crucial for evaluating competing technologies.
- The model also can illustrate process bottlenecks to help guide research.

ARTICLE INFO

Article history:
Available online xxxx

Keywords:
Biorenewables
Chemicals
Technoeconomic
Spreadsheet
Ethanol

ABSTRACT

By using cost correlations and standard scale-factors, a spreadsheet-based early-stage cost estimation tool was developed. Named BioPET (Biorenewables Process Evaluation Tool), this tool allows users to specify up to seven primary unit operations – fermentation, separation, three catalytic stages, and purification – along with key parameters for each. BioPET then computes an estimated minimum selling price for the pathway. Model validation was conducted by selecting three molecules (ethanol, succinic acid, and adipic acid), and comparing BioPET's results to literature values and to results from a commercial process design tool. BioPET produced virtually identical prices to the process design tool, although the costs were not identically distributed amongst the categories. BioPET produced estimates that were within 40% of other literature values at low feedstock costs, and within 5% at high feedstock costs.

1. Introduction

Bio-based chemicals represent an opportunity to produce value-added products from sugars. These chemicals are an attractive alternative to biofuels because of their higher market prices compared to biofuels. In a 2004 study, Werpy and Petersen identified ten chemicals that presented the greatest short-term opportunity for bio-based chemical production in the U.S., spurring tremendous efforts to increase the economic viability of these bio-based chemicals (Sánchez et al., 2005; Song and Lee, 2006; Werpy and Petersen, 2004). However, little is known about the economics of producing these value-added bio-based chemicals at commercial scale.

One chemical that does possess a good deal of process information is ethanol due to its large-scale deployment as a 1st-generation biofuel. The broad ethanol literature encompasses process improvements, technoeconomic analyses (TEAs), and life-cycle assessments, and can provide fundamental knowledge to inform studies about other bio-based chemicals (Kwiatkowski et al., 2006). Robust TEA's, in particular, have the ability to illuminate process bottlenecks and to clarify how process alternatives will impact production costs (Oleskowicz-Popiel et al., 2012). Typically, these TEA's require extensive knowledge of process parameters and design details only available during the latter stages of a project. However, early-stage cost estimation is critical to helping companies and applied academic research centers chart a course through translational research and towards economic viability.

As novel metabolic pathways are explored or novel hybrid fermentative-catalytic processes are proposed (Nikolau et al., 2008); comprehensive and accurate process data necessary for detailed TEAs of these operations at full-scale will be years away. And yet, strong evidence regarding the economic viability of a particular chemical is needed early in the process to warrant continued investment of resources. By making simplifying assumptions and estimates for key variables, it is possible to develop an early-stage TEA of novel processes. Strong TEA capabilities exist commercially in tools such as Aspen Process Economic Analyzer and Intelligen SuperPro Designer®, both of which provide estimations of capital and operating costs. But these tools also require a level of detail

* Corresponding author. Tel.: +1 (515) 294 0465.
E-mail address: rajraman@iastate.edu (D.R. Raman).

0960-8524/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.biortech.2013.08.094

Nomenclature

TEA	technoeconomic analysis
PFD	process flow diagram
C_n	new cost for newly sized piece of equipment
S_n	new size of equipment
S_o	size of equipment where previous cost data exists
C_o	cost of equipment where previous data exists
n	empirically-derived cost exponent
V_{fm}	annual volume of fermentation media (m^3)
m_T	annual production of fermentation product (kg)
c_{fm}	final titer of fermentation product (kg/m^3)
FV_{fm}	useable fraction of fermenter volume (%, purchased volume/usable volume)
η_T	mass conversion efficiency (dimensionless, kg final prod./kg fermentation prod.)
MR	mass ratio (dimensionless, molecular weight of final product/molecular weight of molecule produced in fermentation)
N_b	number of annual batches produced
N_d	number of days of plant operation (days)
t_{fm}	total time to complete a fermentation batch (days)
N_{fm}	number of fermenters required
V_{max}	maximum attainable volume in a purchased fermenter (m^3)
N_c	number of centrifuges
t_d	fermentation downtime (hrs, time used for cleaning and refilling)
VE_c	Centrifuge volumetric energy requirement (kWh/m^3 fermentation liquid)
V_m	Maximum attainable size of a centrifuge
AR	adsorption ratio (kg product adsorbed/Mg adsorbent)
K_f	Freundlich coefficient
[A]	concentration of product in solution (kg/m^3)
n	Freundlich exponent
NA	adsorbent needed (Mg)
τ_A	adsorption time constant (hrs^{-1})
Y_A	adsorption yield
m_p	mass of product per batch (kg)
$\$_c$	cost of crystallizer
X	flow rate of crystals (klb hr^{-1})
N_{min}	minimum number of stages
X_b	fraction of product in the bottoms
X_d	fraction of product in distillate
Y_b	fraction of solute in bottoms
Y_d	fraction of solute in distillate
α	relative volatility of product and distillate
N_{actual}	actual number of sieve trays required
ε_{tray}	Murphee tray efficiency
E_e	extraction factor
K_{Di}	distribution coefficient of the product in its respective solvent
E	extract flow rate
R	raffinate flow rate
ϕ_c	fraction of product not extracted

that is typically unavailable at early stages in process evaluation. While preliminary cost evaluation methods have been outlined by several authors (Peters et al., 2003; Turton et al., 2010), the authors are unaware of any widely-available early-stage TEA model or tool for bio-based chemicals. To address this gap, a spreadsheet-based tool was developed to provide early-stage TEAs of bio-based chemicals named BioPET (Biorenewables Process Evaluation Tool). Key criteria used in the development of BioPET were as follow: (1) ease of use, (2) minimal data inputs, (3) results comparable to simplified models implemented in existing cost-modeling software, and (4) simple graphical reporting of estimated minimum selling prices and cost breakdowns. To operate the tool, users need a basic knowledge (or educated guesses) for each unit operation comprising their overall process design of interest. Once developed, BioPET was compared against SuperPro Designer® and results from Patel (2006) for a suite of three chemicals: ethanol, succinic acid, and adipic acid. The objectives of this research were as follow: (1) To develop a tool capable of informing economic decisions regarding new pathways developed for bio-based chemicals, and (2) To evaluate the tool by comparing its output to literature values and to more sophisticated process modeling/design tools.

2. Methods

2.1. Methods for BioPET development

BioPET was designed with the objectives of evaluating multiple processes with (re)construction of new process flow diagrams (PFD) with each new evaluation. With organisms capable of consuming many types of feedstocks, the model remained agnostic to where the feedstock was derived. In doing so, the tool does not consider upstream processes such as starch hydrolysis or pretreatment and hydrolysis of lignocellulosic biomass – these were considered outside the scope of the model and the feedstock price was considered as a lumped parameter to include the costs of the initial source and conversion technology if required. The feedstock can then be directly fed to fermentation or catalysis, and any other subsequent unit operations.

BioPET assumes the following carbon flow: fermentation, followed by a separation stage, followed by up to three catalytic processes, finishing with up to two purification stages with different unit operations allowed within each stage. All stages in the tool can be toggled on and off to allow for process flexibility. The following approach was taken to accommodate inherent complexity of the separation, catalysis, and purification processes while allowing for a relatively simple user interface: The types separation and catalytic methods along with assumptions are listed in the following sections. This shields the user from having to provide full process details that are often not available at early stages of a project. Finally, within the hypothetical plant, BioPET only examines a stream of material consisting of a primary product and solvent. This binary system uses mass balance equations and relationships to characterize all steps post-fermentation. Using a series of inputs, respective assumptions, and equations described in the following sections, process cost estimations can be made.

Unless otherwise specified, a standard scale-factor approach, as embodied in Eq. (1) (Peters et al., 2003), was used to adjust capital costs based on unit operation size.

$$C_n = \frac{S_n}{S_o} \times C_n^n \quad (1)$$

Where, C_n is the new cost for newly sized piece of equipment, S_n is the new size of equipment, S_o is the size of equipment where previous cost data exists, C_o is the cost of equipment where previous data

Please cite this article in press as: Claypool, J.T., Raman, D.R. Development and validation of a technoeconomic analysis tool for early-stage evaluation of bio-based chemical production processes. Bioresour. Technol. (2013), http://dx.doi.org/10.1016/j.biortech.2013.08.094