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A new representation for modeling biomass to commodity chemicals development for chemical process industry

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ABSTRACT

A new representation combining network and stage-gate frameworks to study the impact of capital and research & development (R&D) decisions on the evolution of biomass to commodity chemicals system is presented. The network representation is used to universally express the interconnections between the processing technologies and to track the material flow among them. The stage-gate representation is used to express the discrete nature of technology maturity levels. The corresponding mixed-integer nonlinear program is developed and solved for a case study. In this case study, ethylene and propylene can be produced from naphtha and/or biomass. The results of the sensitivity analysis reveal that the raw material costs are the dominant factors that dictate the optimum investment decisions and production plan for this system.

1. Introduction

Chemical process industry (CPI) has been highly dependent on fossil-based feedstocks. According to the 2006 Manufacturing Energy Consumption Survey (MECS), CPI consumes as much as 5149 trillion Btu of energy, which accounts for about 24.4% of the total U.S. manufacturing sector energy consumption (U.S. Energy Information Administration, 2009). Of the 5149 trillion Btu, 54.6% is in the form of feedstock (U.S. Energy Information Administration, 2009). As fossil-based reserves deplete, the discovery of alternative feedstocks becomes necessary (Dodds & Gross, 2007). Biomass holds a great potential to be a substitute because it is abundant, locally available, and renewable. Processing biomass to commodity chemicals can be done thermo-chemically (e.g., gasification, pyrolysis, and liquefaction/hydro-thermal upgrading) and bio-chemically (e.g., fermentation and aerobic/anaerobic digestion). These processes are thoroughly reviewed in (Corma, Iborra, & Velty, 2007; Dodds & Gross, 2007; Holladay, White, Bozell, & Johnson, 2007;Werpy, Holladay, & White, 2004).

Incorporating this relatively new feedstock to our existing CPI will require significant amounts of investments mainly for two purposes. First one is to increase the efficiency of the technologies that can be used to convert biomass to commodity chemicals, and hence make them cost competitive to support the CPI system. The second purpose is to expand the production capacities of these technologies to meet the current and future market demands. How these investments will shape the evolution of the biomass-to-commodity-chemicals (BTCC) system should be investigated. For such a study, a mathematical model that can be used to determine the timing and the amounts of R&D and production-capacity expansion investments that will satisfy a predetermined objective, such as the minimum cost, is necessary. Such model, i.e., the BTCC investment planning model, will provide rapid generation of different BTCC system evolutions for the planning horizon resulting from various scenarios generated by modifications of model parameters. Through sensitivity analysis, such a model will also be able to identify the minimum necessary pace of new BTCC technology developments in order to make biomass a significant contributor as a CPI feedstock. Hence, the model and the analysis of the scenarios can be used to assist management decisions and policy development particularly for BTCC technology development for CPI and energy industry.

The BTCC investment planning model should include two aspects of the BTCC system: (1) an ability to outline the connections among the technologies and to track the material flow within them, and (2) an ability to express the discrete technology maturity levels explicitly.

The capability to express the technology map along with the material flow is similar to all network flow problems addressed in process systems engineering literature, and network-style representations that are based on graph theory. The network-based representations, STN, SEN, RTN, GMF, UOPSS, and Group Contribution Method, have been used to express technology interconnections for many systems and track the corresponding material flow within. Most of these representations, when used

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Nomenclature

Indices

a_i	input material nodes for technology e with m inputs, $i \in [1,m]$
c_j	output materials for technology e with n outputs, $j \in [1,n]$
d_e	delivering node for technology e with multiple one input and/or output
e	technologies and pseudo-arcs
i	annual discount factor
in_i	input transfer pseudo-arcs for technology e with m inputs, $i \in [1,m]$
$main_e$	the main arc of technology e with multiple input and/or output
o_j	output pseudo-arcs for technology e with n outputs, $j \in [1,n]$
r_e	receiving node for technology e with multiple input and/or output
s	maturity stages
t	time
v	materials and pseudo-nodes

Sets

A_e	the set of input material nodes for technology e with m inputs, $i \in [1,m]$
C_e	the set output materials for technology e with n outputs, $j \in [1,n]$
E	the set of technologies and pseudo-arcs
In_e	the set of input transfer pseudo-arcs for technology e with m inputs, $i \in [1,m]$
O_e	the set of output pseudo-arcs for technology e with n outputs, $j \in [1,n]$
$Sadv$	the set of advancement stage (in this work, $Sadv = \{3\}$)
V	the set of materials and pseudo-nodes
VP	the set of products
VR	the set of raw materials
VRR	the set of renewable raw materials

Parameters

B	the weighted incident matrix to express the overall interconnections of materials and technologies
$b_{v,e}$	the component of weighted incident matrix B for directed-arc e and node v
$CC_{e,0}$	initial expansion cost of technology e
$CR_{v,0}$	initial cost of material v, $\forall v \in VR$
$CR_{v,t}$	cost of the renewable material v at time t, $\forall v \in VRR$
$CRD_{e,0}$	initial total R&D expenditure of technology e
$CX_{e,0}$	initial cumulative capacity of technology e
$D_{v,t}$	demand of material v at time t, $\forall v \in VP$
IR	inflation rate
k_v	extraction coefficient of nonrenewable materials v, $\forall v \in VR \wedge v \notin VRR$
MW_{a_i}	the molecular weight of material a_i, $i \in [1,m]$
MW_{c_j}	the molecular weight of material c_j, $j \in [1,n]$
$q_{i,i'}$	the production ratio between input material c_j and $a_{j'}$
$Smax$	the highest level of maturity stage (in this work, $Smax = 4$)
$Xmax$	maximum attainable capacity expansion
α_e	learning-by-doing elasticity of technology e
β_e	learning-by-searching elasticity of technology e
γ_v	annual rate of increase for the demand of material v, $\forall v \in VP$
λ_i	the stoichiometric coefficient of input material a_i, $i \in [1,m]$
$\theta_{i,i'}$	the production ratio between input material a_i and $a_{i'}$
ϑ_j	the stoichiometric coefficient of output material c_j, $j \in [1,n]$
η_e	yield of technology e

Variables

$CC_{e,t}$	expansion cost of technology e at time t
$CR_{v,t}$	cost of the nonrenewable material v at time t, $\forall v \in VR \wedge v \notin VRR$
$CX_{e,t}$	cumulative capacity of technology e at time t
$CRD_{e,t}$	total R&D expenditure of technology e at time t
$P_{e,t}$	production of technology e at time t
$R_{v,t}$	amount of material v produced ($\forall v \in VP$) or consumed ($\forall v \in VR$) at time t
TC	total cost
$X_{e,t}$	capacity expansion of technology e at time t
$Y_{e,s,t}$	binary variable of the maturity of technology e, at stage s, at time t

in a continuous-time formulation, assume that the capacities of the processes in these systems do not change with time. Some are process-dependent, and hence, addition of new or removal of obsolete processes/technologies may require significant modifications to the overall problem formulation. But more importantly, network-style representations do not track different maturity levels of the processes within a system. In addition to technology interconnections and material flow, the BTCC system includes technologies that are at different maturities. The investment planning model should be able to track these maturity stages and the pace of each technology marching through these stages explicitly. A technology goes through several maturity stages (e.g., research and pilot-plant stages) before starting to contribute fulfilling the demand. The progression of a technology through different maturity stages is analogous to the march of new products through an R&D pipeline or a stage-gate framework. However, the products or technologies going through the stages are generally independent of each other (Sadin, Povinelli, & Rosen, 1989; Varma, Reklaitis, Blau, & Pekny, 2007). Furthermore, the stage-gate framework alone is not able to track material flow among interconnected technologies. Because the technologies in the BTCC system are interconnected, and the material flow between these technologies should be tracked, stage-gate framework alone would not be enough to model the investment planning problem.

There have been a vast number of studies on conceptual design, process simulation, and techno-economic analysis of integrated biorefineries. A review of these studies for thermochemical pathways is recently compiled by Floudas, Elia, and Baliban (2012). As an example, Bao, Ng, Tay, Jiménez-Gutiérrez, and El-Halwagi (2011) proposed a chemical species/conversion technologies (which are the operators) structural representation. The operators are used to determine the chemical species that can be produced using the specified biomass feedstock and their corresponding pathways. Then, the set of pathways that will satisfy a predetermined objective is identified using an optimization formulation. In another study, Zondervan, Nawaz, de Haan, Woodley, and Gani (2011) developed a biorefinery model using transshipment models coupled with a superstructure. Biorefinery model was optimized to determine the optimum production routes of ethanol, butanol, and