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Modeling Next Generation Feedstock Development for Chemical Process Industry

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Abstract

A new network representation to study the impact of capital and research & development (R&D) investment decisions on the evolution of biomass to commodity chemicals technologies is presented. The corresponding mathematical programming formulation is developed. The model is solved for a simplified ethylene production scenario to demonstrate its ability to predict the capacity expansion and R&D investment decisions.

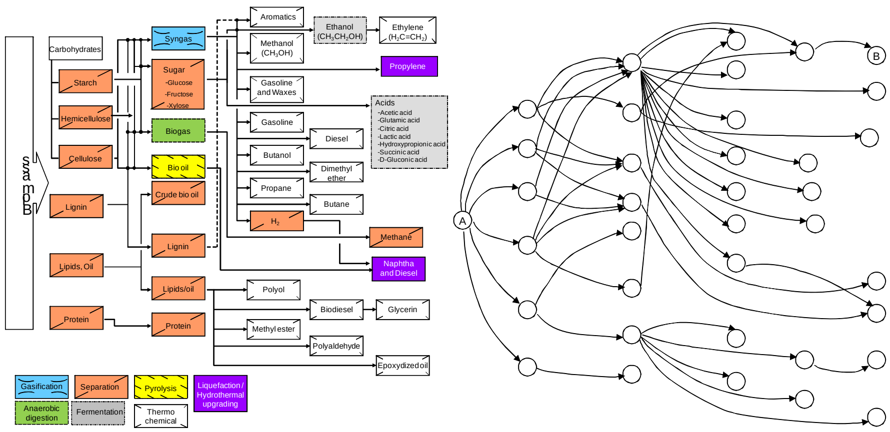
Keywords: biomass to commodity chemicals, optimization, technology evolution.

1. Introduction

Biomass, as a renewable and locally available resource, has great potential for weaning the chemical process industry (CPI) from fossil based feedstocks. There are many different routes to transform biomass into feedstock for the bulk chemicals production. Similar to the use of biomass for fuel production, the technologies for bulk chemicals production can be classified under two main categories: thermo-chemical conversions and bio-chemical conversions. Thermo-chemical conversions are gasification, pyrolysis and liquefaction/hydro-thermal upgrading of the biomass, whereas bio-chemical conversions are fermentation and anaerobic digestion. Figure 1(a) gives a simplified overview of the biomass to commodity chemicals (BTCC) routes that are currently under consideration. Figure 1(a) is not comprehensive; rather the purpose here is to highlight the complexity of the decision space and its interconnections. Reviews of chemicals via bio- and thermo-chemical conversions can be found in (Werpy and Petersen 2004; Kamm, Gruber et al. 2006; Corma, Iborra et al. 2007; Holladay, Bozell et al. 2007; Kamm and Kamm 2007; Haveren, Scott et al. 2008).

The switch from our current fossil fuel based CPI to a future CPI that utilizes biomass feedstock requires substantial amounts of R&D and capital investments for technology development. As such there is great need for investigating how these investments will impact the evolution of the biomass feedstock system. Given the vast number of routes that can be utilized to convert BTCC, the decisions of how much to invest in which technologies for the short, medium and long term in the resource-constrained environment of the CPI is a challenging task. Furthermore, a suitable framework which is amenable to support the investment decisions in this field and which can be used to represent and compare different technology options with their maturation levels and possible evolution paths is not available in the literature.

In this paper, a new framework, based on graph theory, is proposed to fulfill this gap. In the following sections, the proposed framework to study the BTCC investment problem is defined in detail followed by the resulting nonlinear programming (NLP) formulation of the investment problem. A simplified case study is presented to demonstrate the application of the proposed framework. Finally, last section provides conclusions and future directions.



(a) (b)

Figure 1. The technologies to transform biomass to commodity chemicals (a) and the corresponding network representation (b)

2. A New Framework to Study BTCC Investment Problem

Drawing analogies to the graph theory, a network representation is developed as a suitable framework which is amenable to support the investment decisions for the BTCC system. In the network representation, nodes correspond to the materials, i.e., biomass, intermediate chemicals, and commodity chemical, and directed-arcs correspond to the technologies. This yields a directed network G = (V, E) with node set V, and arc set E. For example, Figure 1(b) shows the network representation of the BTCC technologies presented in Figure 1(a). Using index v to denote a node, and index e to denote an arc, the following variables are defined for each arc: cumulative capacity (CX_e, cumulative installed capacity of technology e), transportation cost (CC_e, unit capital cost for technology e), efficiency (η_e, the production efficiency of technology e, η_e, ≤1), α_e and β_e are the learning-by-doing and learning-by-searching elasticities of the corresponding technology, respectively. The transportation cost of an arc can be reduced by expending R&D and capital investments. While the R&D investments do not directly impact the cumulative capacity, the capital investments result in capacity expansions. The relationship between the R&D and capital investments, and the transportation cost and capacity is defined using two-factor learning curve expression (Figure 2). Depending on the R&D and capital investment decision of the CPI players and the government, the BTCC network will evolve differently.

Learning curve concept was first introduced by Wright (Wright 1936). Wright observed that the number of direct labor hours it takes to manufacture one unit of a product decreased at a uniform rate as the quantity of the units manufactured doubled. In their most general form, the learning curve models link the cumulative capacity, the output, or the labor to the technology's cost using the main phenomena observed by Wright: cost decreases uniformly as the cumulative learning source doubles. The original learning curves included only the impact of one-factor (such as capacity) on the cost of the technology. These models are used to represent the learning-by-doing. However, the unit cost of a technology also changes with R&D expenditures, especially at the infancy of the technologies. This impact is called learning-by-searching, and resulted in two-factor learning curves (Kouvaritakis, Soria et al. 2000).

3. Modeling the Evolution of BTCC Technologies

Using the framework described in this paper, the evolution of BTCC technologies is modeled with an NLP. There are three subsets of nodes that are used in the formulation: Raw materials, $VR = \{v|v \in V \wedge v$ is a source node$\}$; Biomass, $VRR = \{\text{biomass}\}$; Products, $VP = \{v|v \in V \wedge v$ is a sink node$\}$. The connectivity of the graph is represented by a weighted incidence matrix, B, which is a $|V|\times|E|$ matrix $B = (b_{v,e})$ (see Figure 2 for the elements of B). It is assumed that the demand for the products increases over time with an annual rate, the cost of biomass increases according to the inflation rate and the cost of nonrenewable raw materials increases linearly with the total resource depletion. With these assumptions, the resulting NLP formulation is given in Figure 2.

4. Case Study

A simplified case study, the evolution of ethylene production from biomass (corn grain + corn stover) through two different technologies compared to conventional ethylene production from naphtha, is presented to illustrate the capabilities of the proposed approach. The network representation of the problem can be seen in Figure 3(a) and the evolution of the resulting production landscape is given in Figure 3(b). The evolution of the ethylene production technologies and production capacities was modeled for a 50 year period. Technology parameters are in Table 1. Initial raw material costs for biomass (grain+stover) and naphtha are assumed to be \$262/dry ton and \$685/ton. The model was solved using GAMS 23.4 – CONOPT in 0.15 CPU seconds. With the model parameters used, the production shifts to utilizing biomass as the technology capacities become available and the only new capacity expansions are biomass utilizing technologies (Figure 3(b)).

Table 1. Technology parameters

Tec, e	η *(wt%)*	α	β	*Initial Cost*	*Initial Capacity (10^6 tons)*
(1)	0.25	-0.20	-0.07	\$0.20/kg	45
(2)	0.80	-0.28	-0.05	\$10.0/kg	0.01
(3)	0.30	-0.20	-0.07	\$10.0/kg	0.01
(4)	0.55	-0.20	-0.07	\$1.0/kg	0.01
(5)	0.25	0.00	0.00	\$1.2/kg	28.3

5. Conclusions and Future Directions

5.1. Conclusions

In this work, BTCC investment problem is described and drawing analogies to graph theory, a new network representation for this problem is proposed. Using the proposed representation, the NLP formulation of the investment problem is presented. A simplified case study, the production of ethylene from conventional naphtha cracking and from biomass via two routes, is modeled to demonstrate the application of the framework. The results suggest that the evolution of the BTCC systems can be modeled by the proposed framework.

Objective Function

Min TC

Subject to

Cost Function

$$TC = \sum_{e}\sum_{t} CC_{e,t}\left(CX_{e,t} - CX_{e,t-1}\right) + \sum_{v \in VR}\sum_{t} CR_{v,t}R_{v,t} + \sum_{e}\sum_{t} CRD_{e,t}$$

Technology Costs (Two-factor learning curve)

$$CC_{e,t} = CC_{e,0}\left(\frac{CX_{e,t}}{CX_{e,0}}\right)^{\alpha_e}\left(\frac{CRD_{e,t}}{CRD_{e,0}}\right)^{\beta_e} \qquad \forall t, e$$

Raw Material Costs

$$CR_{v,t} = CR_{v,0} + k_v \sum_{j=1}^{t} R_{v,j} \qquad \forall t, \left\{v \middle| v \in VR \wedge v \notin VRR\right\}$$

$$CR_{v,t} = CR_{v,0}\left(1 + IR\right)^{t} \qquad \forall t, v \in VRR$$

Product Demands

$$D_{v,t} = D_{v,0}(1 + \gamma_v)^{t} \qquad \forall t, v \in VP$$

Meet Product Demands

$$R_{v,t} \geq D_{v,t} \qquad \forall t, v \in VP$$

$$R_{v,t} = \sum_{e} b_{v,e}P_{e,t} \qquad \forall t, v \in VP$$

No Accumulation of Intermediates

$$\sum_{e} b_{v,e}P_{e,t} = 0 \qquad \forall t, \left\{v \middle| v \notin VP \wedge v \notin VR\right\}$$

Raw Material Requirements

$$R_{v,t} = \sum_{e} -b_{v,e}P_{e,t} \qquad \forall t, v \in VR$$

Capacity Constraints

$$P_{e,t} \leq CX_{e,t} \qquad \forall t, e$$

Capacity and R&D Stock Bounds

$$CX_{e,t-1} \leq CX_{e,t} \qquad \forall t, e$$

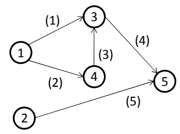
$$CRD_{e,t-1} \leq CRD_{e,t} \qquad \forall t, e$$

Nomenclature

TC: Total cost
$CC_{e,t}$: Unit capital cost for technology e at time t
$CX_{e,t}$: Cumulative installed capacity of technology e at time t
$P_{e,t}$: Amount of production with technology e at time t
$CR_{v,t}$: Unit cost of material v at time t (only defined for raw materials, i.e., source nodes)
$R_{v,t}$: Amount of material v produced or consumed at time t
$CRD_{e,t}$: Total R&D expenditure for technology e at time t
k_v: Constant cost increase coefficient for material v (defined for nonrenewable raw materials)
IR: Inflation rate
$D_{v,t}$: Demand for material v at time t (only defined for products, i.e., sink nodes)
γ_v: Annual increasing rate of demand for material v

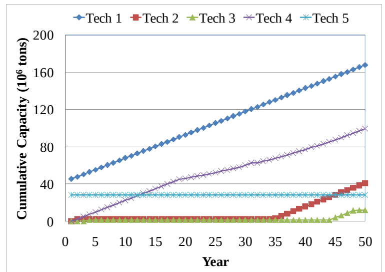
$$b_{v,e} = \begin{cases} -1/\eta_e & \text{if material } v \text{ is a raw material for technology } e \\ 1 & \text{if material } v \text{ is produced by technology } e \\ 0 & \text{otherwise} \end{cases}$$

Figure 2. The NLP formulation of BTCC technologies evolution



Nodes, *v*	Edges, *e*
1 → Biomass	(1) → Fermentation
2 → Naphtha	(2) → Gasification
3 → Ethanol	(3) → Catalytic conversion
4 → Syngas	(4) → Catalytic dehydration
5 → Ethylene	(5) → Cracking

(a)



(b)

Figure 3. The network representation of case study (a) and the resulting cumulative capacity (b)

5.2. Future Directions

The solutions of the model are sensitive to the data used to construct the model. Therefore, a systematic sensitivity analysis will be performed to study the impact of model parameters on the evolution of the BTCC system and on the emergence of the "winner" technologies.

The elasticities in learning-curve equation are usually determined through historical data by regression, hence the elasticities are normally distributed uncertain variables (Gritsevskyi and Nakicenovi 2000). For new technologies the uncertainty in the elasticity estimates will be higher due to the limited amount of data, i.e., the mean of the normal distribution might shift and the variance of the distribution will shrink as more data becomes available. Furthermore, the possible evolution paths of the technologies are dependent on the investment decisions of the individual CPI players as well as the decisions of the government. This is a stochastic optimization problem with endogenous and exogenous uncertainty, because the decisions may impact the distribution parameters and/or the observations of the uncertainties. We will investigate simulation-based optimization approaches to the stochastic BTCC investment problem.

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