STAGE-GATE REPRESENTATION OF FEEDSTOCK DEVELOPMENT FOR CHEMICAL PROCESS INDUSTRY

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Abstract

Utilization of biomass as a feedstock in chemical process industry (CPI) will require investments in research & development (R&D) as well as for capacity expansions. To study the effects of these investments on the evolution of biomass to commodity chemicals (BTCC) system, a new Stage-gate Representation is introduced to complement the network representation presented in Cremaschi (2011). The BTCC evolution is modeled as a mixed integer nonlinear programming and the model is applied to a case study of acetic acid production in order to demonstrate its ability to predict the capacity expansion and R&D investment decisions, and to explicitly include each technology maturity stage.

Keywords

Biomass to commodity chemicals, Stage-gate representation, Technology evolution, MINLP model

Introduction

The chemical process industry (CPI) is a large consumer of fossil fuels mostly in the form of natural gas, liquefied petroleum gas and natural gas liquids. According to the 2006 Manufacturing Energy Consumption Survey (MECS) conducted by U.S. Energy Information Administration, the total net energy consumption of CPI was estimated at 5,149 trillion Btu, which accounts for about 24.4% of the total U.S. manufacturing sector energy consumption (U.S. Energy Information Administration 2009). Of the 5,149 trillion Btu, the CPI utilized about 54.6% as feedstock (U.S. Energy Information Administration 2009). As fossil fuel reserves deplete, alternative feedstocks will be needed to ensure the CPI viability (Dodds and Gross 2007). Due to its abundance, local availability, and renewability, biomass is a promising substitute for fossil feedstocks. Similar to producing fuel from biomass, producing commodity chemicals from biomass can take two main paths of conversion: thermochemical (gasification, pyrolysis, and liquefaction/hydrothermal upgrading) and bio-chemical (bio-chemical conversion are fermentation and anaerobic digestion). These processes are thoroughly reviewed in (Werpy, Holladay et al. 2004; Corma, Iborra et al. 2007; Dodds and Gross 2007; Holladay, White et al. 2007).

Many of these conversion processes have not yet reached the maturity level to support commercial production. In order for these new technologies to reach commercial availability, and to replace and/or supplement the current fossil-based production, R&D investments are necessary. Furthermore, a process will have to have enough installed production capacity to support the market needs implying capital expansion investments. As such there is great opportunity for investigating how these investments will impact the evolution of the biomass feedstock system.

In the following section, we present problem description followed by the details of the Network and Stage-Gate Representations for the BTCC investment problem. Next, the resulting mixed-integer nonlinear

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programming (MINLP) model of the BTCC investment problem is presented followed by a simplified case study to demonstrate the framework application.

Problem Description

Given a number of biomass and fossil-based feedstock processing technologies and their characteristics, and the initial commodity chemicals production system market conditions, the objective is to develop a framework that can be used to formulate an optimization problem to answer the following: how much, to which technology and when to invest in capacity expansions and in R&D to yield a minimum cost commodity chemicals production system over a period of time while incorporating discrete evolution stages of technologies explicitly.

Network Representation

Cremaschi (2011) utilized a network representation to study the BTCC investment problem. In the network representation, the nodes, v, and the directed-arches, e, correspond to the chemical species and the technologies, respectively (Figure 1). Based on the graph theory, the network representation captures the material flow between conversion technologies utilizing all technology efficiencies (Cremaschi 2011), and it incorporates the relationship between the unit cost of a technology and the amount of investments made both in capacity expansions and R&D with two-factor learning curve (Kouvaritakis, Soria et al. 2004). The two factors are the cumulative technology's capacity, $CX_{e,t}$, and the cumulative research investment, $CRD_{e,t}$, at each time. These effects correspond to learning-by-doing and learning-by-searching. The elasticities of the learning-by-doing and learning-bysearching for each technology e are represented by parameters α_e and β_e , respectively. The overall interconnections of the network is expressed via weighted incidence matrix, $B_{v,e}$, elements of which can be defined as

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

where η_e is the yield for technology *e*. Assuming a constant inflation rate for demand and raw material costs, and that the cost of non-renewable feedstock increases as its resource decreases, the network representation was utilized to model the BTCC evolution problem as a nonlinear programming formulation, where the decisions were which technology, how much, and when a capacity expansion and R&D investment should be made to shift the CPI from fossil-based feedstock to biomass feedstock.

Although the network representation is able to capture the material flow between the technologies and the capital and R&D investments' effects on the cost of technologies, it does not capture the technology maturity levels and the fact that a technology first has to reach a certain maturity level to contribute to the production. In this paper, to address these aspects, a new Stage-Gate Representation is introduced to complement and improve the network representation presented in (Cremaschi 2011).



Figure 1. A simple network representation with three species (nodes) and two technologies (directed-arcs)

Stage-Gate Framework for BTCC Investment Problem

The Stage-Gate Framework is inspired by the pharmaceutical R&D pipelines described in (Blau, Pekny et al. 2004) and the Technology Readiness Level metric originally defined by Sadin et al. (Sadin, Povinelli et al. 1989) for assessing the maturity of the technologies within National Aeronautics and Space Administration (NASA). We define a four level metric (consistent with the traditional chemical engineering technology development process.): (1) research stage, (2) pilot plant stage, (3) advancement stage, and (4) commercial stage. A representing schema is given in Figure 2.



Figure 2. Stage-gate Framework for Technology Development

The research stage includes the development of basic principles and proof-of-concept studies in a laboratory scale. It can be assumed that the production capacity using the technology at stage (1) is almost zero. The first scaleup of the technology happens on the pilot plant stage, during which the technology is "validated in a relevant environment" (Sadin, Povinelli et al. 1989). The advancement stage refers to continuous improvement of the technology capabilities while reducing its cost. The demonstration plants are built in this stage and the capacities of these plants can range from 10% of the commercial scale to commercial scale as the cost of the technology decreases. The last stage is the commercial stage. The maturity of each BTCC technology can be represented easily with this four level metrics. At the research stage, a number of new technologies will be suggested and tested at the laboratory scale. Some of these technologies will be successful and move to the pilot plant stage. The number of technologies that move through the gates successfully will decrease with most of the technologies not making it to the advancement stage, and even fewer reaching the commercial stage. Logically, it

follows that a technology can contribute to the production after it reaches stage (3), the advancement stage.

MINLP Model with the Stage-Gate Representation

The MINLP formulation combining Stage-Gate Representation with the network formulation is given in Figure 3. The Stage-Gate Representation constraints are discussed below. The details of the network formulation can be found in (Cremaschi 2011).

The Stage-Gate Representation utilizes a binary variable $Y_{e,s,t}$ to define the maturity level, i.e., the evolution stage, of a technology (Eq. (2)). The subscript *s* represents the defined four level metric, (i.e. stages (1) - (4)):

$$Y_{e,s,t} = \begin{cases} 1 & \text{if technology } e \text{ is at least at stage } s \text{ at time } t \\ 0 & \text{otherwise} \end{cases}$$
(2)

Stage Bracketing constraints, modeled as disjunctions, correlate the cumulative capacity to the evolution stage. *Interstage Preevolution Requirements* make sure that an evolution stage cannot exist unless its previous stages existed. *No Back Evolution* constraint prohibits the progress of technologies in the reverse evolution direction, i.e., from stage (4) to stage (1) with time. A technology can contribute to the production only after it reaches stage (3) (disjunction given as *Capacity Constraints*).

Case Study

A simplified case study of acetic acid production from biomass (starch and lignocellulosic sources) and naphtha is presented in this paper to illustrate the capabilities of our approach. This case study is an extension of the one given in (Cremaschi 2011). The extension also demonstrates the flexibility of the network framework to accommodate new technologies and materials, i.e., it attests to the ease of its re-usability and ease of update of the formulation.

The network representation of the case study is given in Figure 4. Biomass can be processed via fermentation or gasification to produce methanol or syngas, respectively. Naphtha can be gasified, cracked, or oxidized to produce syngas, ethylene, or acetic acid, respectively. Syngas can be converted catalytically to either ethanol or methanol, and ethanol can be dehydrated into ethylene or fermented into acetic acid. Ethylene is converted to acetic acid via the efficient one-step oxidation and methanol can be used to produce acetic acid via carbonylation process.

The efficiency, learning-by-doing and learning-bysearching elasticities, initial cost and initial capacity of the technologies used in the MINLP formulation is given in Table 1. For technologies (1) - (5), the parameters are the ones used by Cremaschi (2011), except for the learningby-doing elasticities for technologies (1), (3), and (4). These learning-by-doing elasticities were obtained by fitting the historical data of the unit production cost of ethanol from sugar cane in Brazil as a function of total production

Objective Function Min TC Subject to Cost Function $TC = \sum_{e,t} \sum_{e,t} CC_{e,t} \ (CX_{e,t} - CX_{e,t-1})$ $+\sum_{v \in VR} \sum_{t} CR_{v,t} R_{v,t} + \sum_{e} \sum_{t} CRD_{e,t}$ Technology Costs $CC_{e,t} = CC_{e,0} \left(\frac{CX_{e,t}}{CX_{e,0}}\right)^{\alpha_e} \left(\frac{CRD_{e,t}}{CRD_{e,0}}\right)^{\beta_e} \quad \forall t, e$ **Raw Material Costs** $CR_{v,t} = CR_{v,0} + k_v \sum_{i=1}^{t} R_{v,j} (1 + IR)^t$ $\forall t, \{v \mid v \in VR \land v \notin VRR\}$ $CR_{v,t} = CR_{v,0} (1 + IR)^t \quad \forall t, v \in VRR$ Product Demands $D_{v,t} = D_{v,0} \left(1 + \gamma_v\right)^t \quad \forall t, v \in VP$ Meet Product Demands $R_{v,t} \geq D_{v,t}$ $\forall t, v \in VP$ $R_{v,t} = \sum b_{v,e} P_{e,t} \quad \forall t, v \in VP$ No Accumulation of Intermediates $\sum b_{v,e} P_{e,t} = 0$ $\forall t, \{v \mid v \notin VP \land v \notin VR\}$ **Raw Material Requirements** $R_{v,t} = \sum_{e} -b_{v,e} P_{e,t} \quad \forall t, v \in VR$ Capacity Constraints $\begin{bmatrix} Y_{e,3,t} \\ P_{e,t} \leq CX_{e,t} \end{bmatrix} \lor \begin{bmatrix} \neg Y_{e,3,t} \\ P_{e,t} = 0 \end{bmatrix} \quad \forall t, e$ Capacity and R&D Stock Bounds $CX_{e,t-1} \leq CX_{e,t} \qquad \forall t, e$ $CRD_{e\,t-1} \leq CRD_{e\,t} \quad \forall t, e$ Interstage Preevolution Requirements $Y_{e,s,t} \le Y_{e,s-1,t} \quad \forall t, e, \{s \mid s \in \{2,3,4\}\}$ No Back Evolution $Y_{e,s,t} \ge Y_{e,s,t-1} \quad \forall t, e, s$ Stage Bracketing $\begin{bmatrix} Y_{e,s,t} \\ CX_{e,t} \ge LO_s \end{bmatrix} \lor \begin{bmatrix} \neg Y_{e,s,t} \\ CX_{e,t} \ge 0 \end{bmatrix} \quad \forall t, e, s$ $CX_{e,t} \le \max(HI_s) \qquad \forall t, e, \{s \mid Y_{e,s,t}\}$

Figure 3. The MINLP formulation of BTCC technologies

evolution (with the Stage-gate Framework addition) capacity as shown in (Ferreira 2002). Technologies (6), (7), (8), and (11) can be assumed to be at the commercial stage and hence, their learning elasticities are set to zero. The yields of technologies (6), (7), (8), (9-10) and (11) are from (Hemminger and Westfield 1944), (Ren, Li et al. 2003), (Tembe, Patrick et al. 2009), (Plotkin and Song 2003), and (Zimmerschied 1978), respectively.



Figure 4. The Network Representation of the Case Study

The learning-by-searching elasticity of technology (9) is set to zero because producing acetic acid from alcohol by fermentation is a very well-known and commercial technology in the food industry. However, its learning-bydoing elasticity is not set to zero, because we postulate that the technology modifications needed to support much higher production rates required for the commodity chemicals industry will come from capacity expansions. The initial capacity is assumed to be small due to the same reason. The unit production cost, \$0.73 per kg (a slightly higher value than the market price of vinegar), is not as large as other undeveloped technologies. The lower progress ratio for technology (9) (compared to technology (1) (a similar technology)) reflects the fact that it will require higher capacity expansions to reduce the unit production cost of this technology. The learning elasticities, and initial cost and capacity of technology (10) are set to be equal to technologies (3) and (4), assuming analogous capacity expansion R&D investment impacts on cost given their similar maturation levels. The initial production costs of technologies (6) and (11) are assumed to be equal to that of technology (5) because these technologies utilize naphtha as the feedstock and they can be easily integrated to the current petroleum refinery industry. The initial unit production cost of technology (7) and (8) are the acetic acid production cost given in (Wagner Jr. 2007). The technology (7) initial capacity is obtained from (Bromberg and Cheng 2010) and the value for technology (8) is estimated by multiplying the technology (7) initial capacity with the yield of technology (8). The initial capacity of technology (6) is calculated by dividing the acetic acid demand by the yields of technology (7) and (8). The initial acetic acid demand, 4.68 million tons, is estimated by extrapolating the year 1999 demand (Wagner Jr. 2007) to the year 2010 with an annual demand increase rate of 2.6%. The majority of current acetic acid production is through technology (8), which can cover up between 80% (Office of Industrial Technologies | U.S. Department of Energy 2003) and 90% of the total production (Sanders 2010). We used the average of these two values as the technology-(8) initial capacity. The remainder of the acetic acid production is assumed to be satisfied by the initial capacity of technology (11).

Table 1. Technology Parameters

| | η | | | $CC_{e,0}$ | $CX_{e,0}$ |
|------|--------|-------|-------|------------|---------------|
| Tech | (wt%) | α | β | (US\$/kg) | $(10^6 tons)$ |
| (1) | 0.25 | -0.21 | -0.07 | 0.20 | 45.40 |
| (2) | 0.80 | -0.28 | -0.05 | 10.00 | 0.10 |
| (3) | 0.30 | -0.21 | -0.07 | 10.00 | 0.10 |
| (4) | 0.55 | -0.21 | -0.07 | 10.00 | 0.10 |
| (5) | 0.25 | 0.00 | 0.00 | 1.20 | 28.30 |
| (6) | 0.80 | 0.00 | 0.00 | 1.20 | 12.00 |
| (7) | 0.40 | 0.00 | 0.00 | 0.80 | 8.66 |
| (8) | 0.99 | 0.00 | 0.00 | 0.80 | 8.57 |
| (9) | 0.99 | -0.10 | 0.00 | 1.00 | 0.10 |
| (10) | 0.86 | -0.21 | -0.07 | 10.00 | 0.10 |
| (11) | 0.70 | 0.00 | 0.00 | 1.20 | 0.70 |

The initial raw material costs for biomass and naphtha are \$262/dry ton and \$685/dry ton, respectively. The extraction cost coefficient and inflation rate are 0.01 and 5%, respectively. Table 2 summarizes the stage upper and lower capacities.

Table I1. Stage Lower and Upper Capacities

| Stage | LO | HI | Notes |
|-------|---------------|---------------|-----------------------------|
| 0 | $(10^6 tons)$ | $(10^6 tons)$ | |
| (1) | 0.1 | <1.0 | LO lowest initial capacity |
| (2) | 1.0 | <4.68 | LO ten times of stage (1)'s |
| | | | lower capacity |
| (3) | 4.68 | <28.3 | LO based on initial acetic |
| | | | acid demand |
| (4) | 28.3 | 500 | LO based on naphtha |
| | | | cracking capacity, HI high |
| | | | enough capacity for this |
| | | | problem |

The resulting non-convex MINLP formulation for a planning horizon of 50 years with bi-yearly cost updates has 9402 equations and 5851 variables. The problem was solved in 17, 18 and 633 CPU minutes to 0.05%, 0.03%, and 0.01% relative-gap using GAMS V23.6.2 global solver BARON V9.0.6 with a Dual Intel E5405 2.0 GHz processor and 8 GB RAM memory. The solution obtained with the 0.01% relative-gap is presented in this paper. With the model parameters used, the evolution of technology capacities and the corresponding technology maturity levels for the specified case study are shown in Figures 5 and 6, respectively.

The result of the optimization problem dictates to invest primarily in the biomass gasification (Figure 5) with supporting capacity expansions on syngas to methanol catalytic conversion and methanol carbonylation technologies. The acetic acid production is switched to the cheaper biomass gasification route as this technology matures enough to contribute to the production at year six. The capacity of the biomass gasification technology increases throughout the planning horizon to replace the more costly naphtha gasification technology. During the initial stages of the planning horizon, between years two and five, minor capacity expansions are realized on naphtha gasification and naphtha oxidation technologies to fulfill the increasing market demand for acetic acid.



Figure 5. The Resulting Cumulative Capacity of the BTCC Evolution Problem

The R&D and capacity expansion investments in biomass gasification (technology 2) result in continuous evolution of this technology from stage (1) initially to stage (2) at year two, followed by stage (3) at year six and finally to stage (4) at year 36 (Figure 6). The only other technology that progressed through the stages is naphtha catalytic oxidation (technology 11), which evolves through stage (2) and stage (3) in years two and five due to capacity expansions, respectively. The biomass fermentation (technology 1), the naphtha cracking (technology 5), the naphtha gasification (technology 6), the syngas conversion to methanol (technology 7), and the methanol carbonylation (technology 8) processes stay at their initial maturity stages throughout the planning horizon. Although there have been small capacity expansions for naphtha gasification, syngas conversion to methanol, and methanol carbonylation technologies, they are not big enough to influence the maturity level of these technologies. The technologies that are not shown in Figure 6 stay at stage (1) for the whole planning horizon. In other words, they remain at the research stage and were not selected to support market demand.



Figure 6. The Resulting Maturity Levels or Maturity Stages of the BTCC Evolution Problem

Conclusions and Future Directions

Conclusions

Alternative resources, such as biomass, must be considered for CPI feedstock in lieu of depleting fossilbased resources. To perform this shift, investments in capacity expansion and R&D is unavoidable. In this paper, the BTCC investment problem – the decisions of how much, to which technology, and when to investment in order to ensure the lowest cost transition from our current fossil-based feedstocks to biomass as the feedstock for the CPI –is discussed. In order to study the BTCC problem, a Stage-Gate Representation is introduced to complement the previously developed network representation by Cremaschi (2011). A simplified case study of acetic acid production from biomass and naphtha is presented to demonstrate the applicability of the framework.

The result suggests that the framework is able to show the shift from petroleum sources to biomass as the CPI feedstock. It was also emphasized that the network representation can incorporate new technologies as they become available or as more information is collected. With the addition of Stage-Gate Representation to the network model, the MINLP formulation is not only able to predict the evolution of BTCC technologies following the market needs, but also able to identify the technology maturity levels and to account for the fact that production from any technology can only be realized after reaching a certain maturity level.

Future Directions

The solution of the MINLP formulation is very sensitive to the parameters values; therefore a systematic sensitivity analysis will be performed to investigate the impact of these parameters on the BTCC system evolution.

The learning elasticities are uncertain variables (Gritsevskyi and Nakicenovi 2000) because they are obtained via regression of the historical data. There are also uncertainties in product demands and technology yields. From these uncertainties, with their decision dependent nature learning elasticities and technology yields are endogenous uncertainties, whereas product demand uncertainty can be classified as exogenous. Thus, our future work will focus on incorporating these endogenous and exogenous uncertainties to the BTCC investment problem. We will develop simulation-based optimization (SIMOPT) approaches to study the stochastic BTCC investment problem.

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

 $R_{v,t}$: Amount of material v produced or consumed at time t *CRD_{e,t}*: Total R&D expenditure for technology e at time t $Y_{e,s,t}$: A binary variable, defined as 1 if technology e is at

 $T_{e,s,t}$. A binary variable, defined as 1 in technology e is a least at stage s at time t and 0 otherwise

 k_{v} : Constant cost increase coefficient for material v (defined only for nonrenewable raw materials)

IR: Inflation rate

 $D_{v,t}$: Demand for material v at time t (defined only for products)

 γ_{v} : Annual increasing rate of demand for material v

 LO_s : The lower limit of the cumulative capacity for stage *s* HI_s : The upper limit of the cumulative capacity for stage *s*

VR: Raw material set

VRR: Renewable raw material set (subset of VR)

VP: Products set

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