

4-2014

Integrated supply chain design for commodity chemicals production via woody biomass fast pyrolysis and upgrading

Yanan Zhang

Iowa State University, yananz@iastate.edu

Guiping Hu

Iowa State University, gphu@iastate.edu

Robert C. Brown

Iowa State University, rcbrown3@iastate.edu

Follow this and additional works at: http://lib.dr.iastate.edu/imse_pubs

 Part of the [Industrial Engineering Commons](#), [Mechanical Engineering Commons](#), and the [Systems Engineering Commons](#)

The complete bibliographic information for this item can be found at http://lib.dr.iastate.edu/imse_pubs/55. For information on how to cite this item, please visit <http://lib.dr.iastate.edu/howtocite.html>.

Integrated supply chain design for commodity chemicals production via woody biomass fast pyrolysis and upgrading

Yanan Zhang^a, Guiping Hu^{*b, c} and Robert C Brown^{a, b}

^a Department of Mechanical Engineering, Iowa State University, Ames, IA 50011

^b Bioeconomy Institute, Iowa State University, Ames, IA 50011

^c Industrial and Manufacturing Systems Engineering, Iowa State University, Ames, IA 50011

Abstract

This study investigates the optimal supply chain design for commodity chemicals (BTX, etc.) production via woody biomass fast pyrolysis and hydroprocessing pathway. The locations and capacities of distributed preprocessing hubs and integrated biorefinery facilities are optimized with a mixed integer linear programming model. In this integrated supply chain system, decisions on the biomass chipping methods (roadside chipping vs. facility chipping) are also explored. The economic objective of the supply chain model is to maximize the profit for a 20-year chemicals production system. In addition to the economic objective, the model also incorporates an environmental objective of minimizing life cycle greenhouse gas emissions, analyzing the trade-off between the economic and environmental considerations. The capital cost, operating cost, and revenues for the biorefinery facilities are based on techno-economic analysis, and the proposed approach is illustrated through a case study of Minnesota, with Minneapolis-St. Paul serving as the chemicals distribution hub.

NOTICE: This is the author's version of a work that was accepted for publication in Bioresource Technology. Changes resulting from the publishing process, such as peer review, editing, corrections, structural formatting, and other quality control mechanisms may not be reflected in this document. Changes many have been made to this work since it was submitted for publication. A definitive version was subsequently published in Bioresource Technology, 158, April (2014), doi: [10.1016/j.biortech.2014.01.049](https://doi.org/10.1016/j.biortech.2014.01.049).

Keywords

Supply chain optimization; Commodity chemicals; Fast pyrolysis; Woody biomass

NOTICE: This is the author's version of a work that was accepted for publication in Bioresource Technology. Changes resulting from the publishing process, such as peer review, editing, corrections, structural formatting, and other quality control mechanisms may not be reflected in this document. Changes many have been made to this work since it was submitted for publication. A definitive version was subsequently published in Bioresource Technology, 158, April (2014), doi: [10.1016/j.biortech.2014.01.049](https://doi.org/10.1016/j.biortech.2014.01.049).

1. Introduction

The growing interest in biofuels production has generated much related research in economic analysis, environmental assessment, and supply chain system design (An et al., 2011; Blottnitz and Curran, 2007; Bowling et al., 2011; Giarola et al., 2012; Hamelinck et al., 2005; Hess et al., 2007; Larson, 2006; Stephen et al., 2010; You et al., 2012; Zhang et al., 2013a; Zhang et al., 2013b; Zhang et al., 2013d). Biomass logistics are complicated by the bulky, distributed nature of biomass and by the high volumes of low energy density materials to be collected and transported to the conversion facilities (Tallaksen, 2011). The unique nature of biomass feedstock provides great impetus for the exploration of sustainable and robust supply chain systems.

Numerous studies have been devoted to optimal design and operational planning of the bioethanol supply chain. You et al. (2012) developed a multi-objective mixed integer linear programming (MILP) model which addressed the optimal design and planning of the cellulosic ethanol supply chain under economic, environmental, and social objectives. Dunnett et al. (2008) proposed a system model to optimize the lignocellulosic bioethanol supply chain under assumptions of energy integration. Bai et al. (2011) optimized biofuel refinery location and supply chain planning for bioethanol production, taking into account of traffic congestion issues. Giarola et al. (2012) developed a stochastic modeling framework adopting a scenario-based approach to assess the effects of trading greenhouse gas (GHG) emissions allowances under market uncertainty for bioethanol production.

Researchers have also been aggressively exploring the supply chain design for biomass-derived transportation fuels (gasoline and diesel fuel). You et al. (2011) presented the optimal design and planning of a biomass-to-liquids (BTL) supply chain under economic and environmental criteria. You's design was based on a distributed preprocessing and centralized conversion network. Kim et al. (2011) designed an optimal biomass supply chain network for transportation fuels production under uncertainty and then analyzed the robust design with Monte Carlo simulation. Elia et al. (2013) developed a nationwide supply chain optimization framework for a BTL system using hardwood biomass for gasoline, diesel, and jet fuel production.

While much research is devoted to the use of biomass for fuels, there has been a concurrent growing interest in the use of biomass for the biobased products, such as renewable chemicals (Brehmer et al., 2009; Christensen et al., 2008; Dale, 2003; Gavrilescu and Chisti, 2005; Schilling, 1995). A survey on the alternative feedstocks for commodity chemicals manufacturing was conducted by Oak Ridge National Laboratory (2007) and biomass was recognized as one of the most promising alternative feedstocks for commodity chemicals production. Various production pathways, such as gasification, fermentation, and pyrolysis, were analyzed. Brehmer et al. (2009) evaluated the maximum fossil fuel replacement potential for a variety of feedstocks and reported a high potential for biomass to replace fossil fuel in the petrochemical industry. Christensen et al. (2008) discussed the possibility of establishing a renewable chemicals industry and reported that from both economic and ecological perspectives, such an industry might be most advantageous to secure the optimal use of abundant, but limited, bioresources.

Vispute et al. (2010) proposed a novel integrated catalytic thermochemical pathway to convert woody biomass to commodity chemicals, such as benzene, toluene, and xylene aromatic hydrocarbons (BTX). In this pathway, the bio-oil produced from woody biomass fast pyrolysis undergoes two-stage hydrotreatment followed by fluid catalytic cracking (FCC). Due to the high selectivity of commodity chemicals products attainable using this production pathway, the pathway has garnered significant attention and has inspired further examination of its economic feasibility and environmental effects. A techno-economic study has been conducted to examine the five commodity chemicals production scenarios, one of which was Vispute's two-stage hydrotreating followed by FCC. Vispute's pathway is found to be the most profitable among the five scenarios (Brown et al., 2012). Another techno-economic study concluded that this chemicals production pathway is economically feasible, in which the facility internal rate of return was predicted to be as high as 13% for a 20-year project (Zhang et al., 2013b). A life cycle assessment was conducted to examine the environmental performance and found that chemicals production via the integrated catalytic processing pathway could reduce GHG emissions significantly compared to the petroleum-based chemicals production (Zhang et al., 2013c).

Although there have been many studies of supply chain design and optimization for biofuel production, there have been few papers addressing supply chain design and optimization for renewable chemicals production from woody biomass via the thermochemical pathway. In this paper, a supply chain network is designed and optimized for the biobased chemical production pathway, using MILP modeling to

optimize the locations and capacities of distributed preprocessing hubs and centralized biorefinery facilities. This paper examines both economic and environmental criteria in a multi-objective framework that allows analysis of trade-offs between economic feasibility and environmental impact. A case study for the state of Minnesota is presented to illustrate the integrated supply chain network design model.

2. Materials and Methods

2.1 Integrated catalytic processing pathway

Vispute et al. (2010) has proposed an integrated catalytic processing pathway for commodity chemicals production via woody biomass (Figure 1). In this pathway, woody biomass is preprocessed (chopped, dried, and grinded) and then sent to a pyrolyzer to produce bio-oil. The bio-oil undergoes phase separations through a liquid-liquid extractor, resulting in separate water insoluble and aqueous phases. The water insoluble phase consists mainly of pyrolytic lignin, which is treated as a co-product. The aqueous phase is sent to a low temperature hydrotreating process (125°C, 100 bar). Then the hydrotreated bio-oil is sent to a high temperature hydrotreating process for further hydrodeoxygenation (200°C, 100 bar) over catalysts. After the two-stage hydrotreating process, FCC is performed on the hydrotreated aqueous phase to produce commodity chemicals. In addition to the primary raw material the woody biomass, hydrogen is needed for the two-stage hydrotreating process. Hydrogen is produced through the steam reforming of natural gas. Natural gas usually contains sulfur, so the gas goes through a desulfurizer for purification before entering the steam methane reformers and water gas shift reactors. The produced hydrogen is then separated from the syngas and send to the hydrotreaters.

{Insert Figure 1 here}

2.2 Supply chain model description

In this paper, the optimal plant sizes, locations, biomass and product flows are considered as the decision variables for the integrated supply chain design. **Table A1(in the appendix)** shows descriptions for decision variables and the parameters for the economic and environmental objectives.

{Insert Table 1 here}

Figure 2 illustrates the supply chain network schematics for chemicals production via woody biomass fast pyrolysis and upgrading. First, the woody biomass is harvested and collected from location i . Two types of woody biomass are considered: raw forest residue and the residue chipped with a road-side chipping method. Both woody biomass types need to be preprocessed for size and moisture reduction before conversion. For biomass preprocessing, two methods are considered. One method is distributed preprocessing, where multiple preprocessing centers are located close to biomass sources. The other method is integrated preprocessing, where the biomass is gathered into one integrated facility. The integrated facility has a preprocessing facility and the biorefinery facility. All the preprocessing facilities are to chop, dry, and grind the biomass to reduce the moisture and sizes. Then the preprocessed biomass is sent to the biorefinery facilities. Chemicals and co-products are produced at the integrated facility location. The co-products are char and lignin which are left at the local location and the chemicals are transported to the distribution center.

{Insert Figure 2 here}

2.3 Model formulation

2.3.1 Economic objective

The economic objective is to maximize the net present profit for a 20-year project producing commodity chemicals via woody biomass fast pyrolysis and upgrading:

$$\max \sum_{a=1}^n \varphi_a (R_a - Va - F - C - T - P) - P_0 \quad (1)$$

The R_a is a function of the annual revenue R_a , annual variable

R_a

operating cost (Va), annual fixed operating cost (F), annual biomass collection cost (C), annual biomass transportation cost (T), the plant capital cost (P_0) and the discount factor (φ_a).

The discounted factor φ_a is used to calculate the net present. Annual interest r is assumed to be 10% for the 20-year project (2011-2032). The discount factor is shown below:

$$\varphi_a = \frac{1}{(1+r)^{t-1}} \quad (2)$$

The annual revenue R_a is the sum of the revenue from chemicals product and

R_{co}

the revenue from the co-products at individual plant location in year t as described in

Equation 3. The annual revenue is not same for every year since the selling price of the

chemical product m in year t ($P_{m,t}$) is assumed to be changing every year. The prices

of chemicals throughout the years are predicted based on EIA petroleum price prediction.

$$V_{m,t} = \sum_{i=1}^n \sum_{j=1}^n V_{i,j} P_{m,t} + \sum_{i=1}^n \sum_{j=1}^n V_{i,j} P_{m,t} \quad (3)$$

The annual variable operating cost $V_{m,t}$ is a sum of variable operating costs for the distributed preprocessing facilities, integrated preprocessing facilities, and integrated biorefinery facilities, which is shown in Equation 4. The variable operating costs include the costs for plant operation, such as electricity, process water, and catalysts.

$$V_{m,t} = \sum_{i=1}^n V_{i,t} P_{m,t} + \sum_{i=1}^n \sum_{j=1}^n V_{i,j} P_{m,t} + \sum_{i=1}^n \sum_{j=1}^n V_{i,j} P_{m,t} + \sum_{i=1}^n \sum_{j=1}^n V_{i,j} P_{m,t} + \sum_{i=1}^n \sum_{j=1}^n V_{i,j} P_{m,t} \quad (4)$$

The annual fixed operating cost $F_{m,t}$ is defined by Equation 5. The fixed operating cost includes the salaries, overhead, and maintenance costs for the distributed preprocessing facilities and integrated facilities.

$$F_{m,t} = \sum_{i=1}^n F_{i,t} + \sum_{i=1}^n \sum_{j=1}^n F_{i,j} \quad (5)$$

(5)

◆◆◆

The annual biomass collection cost C_{bc} is the sum of collection costs for raw biomass and roadside chipped biomass given in Equation 6.

$$\begin{aligned}
C_{bc} = & \sum_{i=1}^n \sum_{j=1}^m \left(C_{bc,raw} + C_{bc,chip} \right) + \sum_{i=1}^n \sum_{j=1}^m \left(C_{bc,raw} + C_{bc,chip} \right) + \sum_{i=1}^n \sum_{j=1}^m \left(C_{bc,raw} + C_{bc,chip} \right) + \sum_{i=1}^n \sum_{j=1}^m \left(C_{bc,raw} + C_{bc,chip} \right) \quad (6)
\end{aligned}$$

The annual biomass transportation cost $\sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau}$ includes the transportation costs of all of the materials (biomass, chemicals, and natural gas), as shown in Equation 7.

$$\begin{aligned} \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} = & \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \\ & \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \\ & \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \\ & \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \sum_{\tau=1}^T \sum_{i=1}^I h_{i,\tau} \alpha_{i,\tau} + \end{aligned} \quad (7)$$

The plant capital cost, the sum of capital investment for all of the facilities, is assumed to be invested in the current year, so the discount factor is not applied (see Equation 8).

$$\sum_{i=1}^I C_{i,0} = \sum_{i=1}^I C_{i,0} + \sum_{i=1}^I C_{i,0} \quad (8)$$

2.3.2 Environmental objective

The environmental objective for GHG-emissions minimization is defined as follows:

$$\sum_{i=1}^I \sum_{\tau=1}^T E_{i,\tau} = \sum_{i=1}^I \sum_{\tau=1}^T E_{i,\tau} + \sum_{i=1}^I \sum_{\tau=1}^T E_{i,\tau} + \sum_{i=1}^I \sum_{\tau=1}^T E_{i,\tau}$$

where:

$$\sum_{i=1}^I \sum_{\tau=1}^T E_{i,\tau} = \sum_{i=1}^I \sum_{\tau=1}^T h_{i,\tau} \alpha_{i,\tau} + \sum_{i=1}^I \sum_{\tau=1}^T h_{i,\tau} \alpha_{i,\tau} + \sum_{i=1}^I \sum_{\tau=1}^T h_{i,\tau} \alpha_{i,\tau} + \sum_{i=1}^I \sum_{\tau=1}^T h_{i,\tau} \alpha_{i,\tau} \quad (9)$$

$$\begin{aligned}
& \sum_{\diamond=1}^{\diamond} \sum_{\diamond} b_{\diamond\diamond\diamond} \\
& \tau_{\diamond\diamond} + \sum_{\diamond=1}^{\diamond} \sum_{\diamond=1}^{\diamond} \tau_{\diamond\diamond\diamond} + \tau_{\diamond\diamond\diamond} + \tau_{\diamond\diamond\diamond} + \tau_{\diamond\diamond\diamond} \\
& \sum_{\diamond=1}^{\diamond} \sum_{\diamond=1}^{\diamond} \tau_{\diamond\diamond\diamond} + \sum_{\diamond=1}^{\diamond} \sum_{\diamond=1}^{\diamond} \tau_{\diamond\diamond\diamond} + \sum_{\diamond=1}^{\diamond} \tau_{\diamond\diamond\diamond} \\
& \tau_{\diamond\diamond\diamond}
\end{aligned}$$

$$+ \sum_{i=1}^n \sum_{k=1}^n \dots \quad (10)$$

$$\dots = \dots + \sum_{i=1}^n \dots + \sum_{i=1}^n \dots + \sum_{i=1}^n \dots + \dots \quad (11)$$

In Equation 9, \dots is the CO₂-equivalent GHG emissions associated with the \dots is the emission of a collection-unit amount of raw biomass collection processes. Here

\dots is the emission of a collection-unit amount of biomass from harvest site i , and

\dots roadside chipped biomass. In Equation 10, \dots is the CO₂-equivalent GHG emissions associated with the materials transportation processes. The term \dots is the emission of a transporting-unit amount of raw biomass, \dots is the emission of a transporting-unit amount of roadside chipped biomass, and \dots is the emission of a transporting-unit amount of preprocessed biomass. The term \dots is the emission of a transporting unit amount of natural gas, and \dots is the emission of a transporting unit amount of chemicals. In Equation 11, \dots is the emissions associated with the biomass conversion processes. Here, \dots is the emission of raw biomass preprocessing process, \dots is the emission of roadside chipped biomass preprocessing process and \dots is the emission of a converting unit amount of preprocessed biomass at biorefinery facility location k .

2.3.3 Biomass supply constraints

In this section, the mass balance of biomass flows and facility capacities constraints are included. The total collected biomass B_i should not exceed the total biomass allowed for

collection in harvesting location i . In Equation 12, α_i is the sustainability factor, which illustrates the allowed collection percentage of the available biomass.

$$B_i \leq \alpha_i B_{i, \text{max}}, \forall i \quad (12)$$

The total collected biomass B_i can be categorized into two types: raw biomass and roadside chipped biomass. They both can be transported to either the distributed preprocessing facility location j or the integrated facility location k . In Equations 13-15,

r_{ij} and h_{ij} are the amount of transported raw biomass and roadside chipped biomass from harvest location i to distributed preprocessing location j . r_{ik} and h_{ik} are the amount of raw biomass and roadside chipped biomass transported from harvest location i to integrated facility location k . ε is the loss factor for the biomass transportation process. B_j is the total received biomass (raw biomass and roadside chipped biomass) in distributed preprocessing facility location j , and B_k is the total biomass (raw biomass and roadside chipped biomass) received in integrated preprocessing facility location k .

$$\sum_{j=1}^J (r_{ij} + h_{ij}) + \sum_{k=1}^K (r_{ik} + h_{ik}) = \alpha_i (1 - \varepsilon) B_i, \forall i \quad (13)$$

$$\sum_{j=1}^J (r_{ij} + h_{ij}) = B_j, \forall j \quad (14)$$

$$\sum_{k=1}^K (r_{ik} + h_{ik}) = B_k, \forall k \quad (15)$$

2.3.4 Distributed preprocessing facility constraints

The distributed preprocessing facility constraints are shown in Equations 16-20.

$$x_{jk} \leq \sum_{l=1}^L a_{jl} \cdot y_{jl} \quad \forall j, k \quad (16)$$

For each candidate location j , there is at most one facility with capacity level l .

$$\sum_{l=1}^L y_{jl} \leq 1, \forall j \quad (17)$$

The total number of distributed preprocessing facilities at location j with capacity level l

should not exceed the maximum number n_{jl} .

$$\sum_{k=1}^K \sum_{l=1}^L y_{jl} \leq n_{jl}, \forall j \quad (18)$$

For equations 8 and 9, the received biomass w_{jk} is preprocessed with a yield α_{jl} of α_{jl} at

distributed preprocessing facility location j and then w_{jk} is transported to the integrated biorefinery location k .

$$w_{jk} = \alpha_{jl} \cdot y_{jl} \quad \forall j, k \quad (19)$$

$$\sum_{l=1}^L y_{jl} = 1, \forall j \quad (20)$$

2.3.5 Integrated facility constraints

The total biomass (raw biomass and roadside chipped biomass) received in integrated preprocessing facility location k is presented as w_k . As indicated in Equation 21, the

received biomass is preprocessed to dry biomass with a yield β_k of β_k at location k . The

total preprocessed biomass B_k is the sum of preprocessed biomass from integrated preprocessing facility B_k^I and that from distributed preprocessing facility $\sum_{l=1}^L B_k^D$, as described in Equation 22. In the integrated biorefinery facility location k , the preprocessed biomass B_k is converted to various chemicals, as shown in Equation 23. μ_m is the conversion rate for specific chemical m , and Q_m is the production quantity of

chemical m at location k . In addition to the chemicals, the co-products pyrolytic lignin and biochar are produced at integrated biorefinery facility. In Equation 24, μ_v is the conversion rate for co-products and Q_v is the production of co-product v at location k .

$$\sum_{l=1}^L B_k^D + B_k^I = B_k, \forall k \quad (21)$$

$$Q_m = \mu_m B_k, \forall k \quad (22)$$

$$Q_v = \mu_v B_k, \forall k \quad (23)$$

$$\sum_{k=1}^K Q_m = \sum_{k=1}^K \mu_m B_k, \forall m \quad (24)$$

The total preprocessed biomass for the integrated biorefinery facility at location k should not exceed the capacity of the integrated biorefinery a_k if facility level l is selected

(Equation 25). At most one facility can exist in one location as indicated in Equation 26.

In Equation 27, the total number of facilities should not exceed the maximum facility

$$\sum_{k=0}^{\infty} a_k \leq \sum_{k=0}^{\infty} a_k, \forall$$

(25)

$$\sum_{i=1}^I 1_{i,k} \leq 1, \forall k \quad (26)$$

$$\sum_{i=1}^I 1_{i,k} \leq 2_{i,k}, \forall k \quad (27)$$

$$i = 1$$

2.3.6 Natural gas and chemicals constraints

In Equation 28, the total natural gas demand at the biorefinery locations is the sum of natural gas flows from various natural gas suppliers. The supplied natural gas from location n to all biorefinery facilities should not exceed the available natural gas in supply location n as indicated in Equation 29. In Equation 30, natural gas demand is calculated

as a factor θ of the preprocessed total biomass $1_{i,k}$ at biorefinery location k . The total

chemicals production $2_{i,k}$ (Equation 31) is the sum of all types of chemical m produced from all of the integrated facility locations. In Equation 32, the total chemicals production should not exceed the maximum chemicals demand.

$$\sum_{i=1}^I 1_{i,k} = 2_{i,k}, \forall k \quad (28)$$

$$\sum_{i=1}^I 1_{i,k} \leq 2_{i,k}, \forall k \quad (29)$$

$$2_{i,k} = \theta 1_{i,k}, \forall k \quad (30)$$

$$\sum_{i=1}^I \sum_{k=1}^K 2_{i,k} = 2_{i,k} \quad (31)$$

$$2_{i,k} \leq 2_{i,k}^a \quad (32)$$

3. Result and Discussion

3.1 Data Sources

In this paper, forest residue is the feedstock and the state of Minnesota is employed for the case study. The amount of available forest residue is obtained from the National Renewable Energy Laboratory (NREL, 2013). Each county in Minnesota is considered as a candidate harvesting site, a potential distributed preprocessing facility location, and potential integrated facility location. The Minneapolis-St. Paul metro area has the most convenient transportation resources; therefore, Minneapolis-St. Paul is selected to be the distribution center. The chemicals demand data are based on the commodity flow survey for Minnesota (BTS, 2007). All of the chemicals are assumed to be transported to the distribution center in Minneapolis-St. Paul. The information about the natural gas suppliers and their gas availability is obtained from the U.S. Energy Information Administration (EIA, 2011).

Five capacity levels (L1, L2, L3, L4, and L5) are considered for distributed preprocessing and integrated facilities; L1, L2, L3, L4, and L5 correspond to 100, 200, 500, 1000, and 2000 metric ton/day dry biomass processing capacities. The 2000 metric ton/day capacity plant is selected as the reference plant and the bio-oil conversion rate is assumed to be 52 wt.% of dry biomass. The capital costs for the distributed and integrated facilities are based on the techno-economic analysis (Brown et al., 2012; Zhang et al., 2013b). A scale factor of $n=0.6$ is employed to estimate the capital costs. In Equation 34, ϕ_{new} and ϕ_0 represent the new plant size and the reference plant size, and ϕ_{new} and ϕ_0 are the capital costs for the new plant and the reference plant.

$$C_{0,pre} = C_0 \left(\frac{C_{new}}{C_0} \right) \quad (34)$$

For biomass preprocessing, two methods are considered. One is to preprocess biomass in distributed preprocessing facilities and the other is to preprocess biomass in integrated preprocessing facilities. **Table A2 (in the Appendix)** details the capital costs and the fixed operating cost for the distributed preprocessing facility and for the integrated preprocessing and biorefinery facility at various levels (Zhang et al., 2013b). The fixed operating cost includes salaries, overhead, maintenance, and insurance. The maintenance fees are assumed to be 6% of the facility capital cost. The overhead and insurance are assumed to be 2% and 1.5% of the total salaries, respectively.

{Insert Table 2 here}

The variable costs for the distributed preprocessing facility and integrated preprocessing facility for same biomass are assumed to be the same. But for raw biomass and roadside chipped biomass preprocessing, variable operating costs are different. For roadside chipped biomass preprocessing process, the variable operating cost does not include chopping cost in **Table A3 (in the Appendix)**. For the environmental impact assessment, all GHG emissions related to biomass collection, materials transportation, and production processes are based on the Aspen Plus, SimaPro and GREET models (Zhang et al., 2013b; Zhang et al., 2013c). The emission for the distributed preprocessing facility and integrated preprocessing facility for same biomass are assumed to be the same. But raw biomass preprocessing and roadside chipped biomass preprocessing have different

emissions. The variable operating costs for facilities and emissions data are derived from the reference plant data (**Table A3**) (Zhang et al., 2013b; Zhang et al., 2013c).

{Insert Table 3 here}

The 2012-2035 chemicals prices are based on the techno-economic analysis (Zhang et al., 2013b). The correlations between each chemical species and petroleum price are used to calculate the prices for the next 20 years. The chemical yield and market prices for the next 20 years are shown in **Table A4 (in the Appendix)**. The co-products yields include char, pyrolytic lignin, and fuel gas. The prices of the co-products are \$18.21, \$22.05, and \$200 per metric ton for char, pyrolytic, and fuel gas respectively.

{Insert Table 4 here}

The collection costs for raw biomass and roadside chipped biomass are based on Leinonen (2004). Forest haulage cost is \$9.8/ton for raw forest residue. The stumpage price for the forest residue is assumed to be \$5/metric ton. So the collection cost for raw biomass is \$15.8 /metric ton. For roadside chipped forest residue, there is a \$9.8/ton haulage cost, \$9.8/ton chipping cost, and stumpage cost of \$5/metric ton. Therefore, the collection cost for roadside chipped forest residue is \$26.6/metric ton.

The costs of the harvesting methods of forest residues also have been reported by Leinonen (2004). The four harvest methods include bundle, terrain chip, road chip, and plant chip. The road transportation costs for raw forest residue and roadside chipped forest residue are \$12.8/ton and \$18.3/ton for 80 km. As calculated, the variable

transportation costs for raw forest residue and roadside chipped forest residue are assumed to be \$0.41/metric-ton-mile and \$0.28/metric-ton-mile. The preprocessed forest residue is transported by the trucks with a fixed transportation cost of \$3.32/metric ton for wood chips loading and unloading and a variable transportation cost of \$0.124/metric-ton-mile (Searcy et al., 2007). The transportation cost of commodity chemicals is assumed to be same as the national average truck shipping cost of \$0.286/metric-ton-mile (BTS, 2012). The transportation cost of natural gas via pipeline is assumed to be same as the national average oil pipeline cost of \$0.0297/metric-ton-mile (BTS, 2012). The distances between counties are based on the great circle distances calculated based on the latitudes and longitudes. Circuitry factors are incorporated to estimate the actual transportation distances. The circuitry factors are assumed to be 1.27 (Rogers and Brammer, 2009) and 1.1 for truck and pipeline, respectively (CBO, 1982). This model employs MATLAB to collect the data and uses geographic information system (GIS) software to map the biomass availability and locations. The mathematical model is coded in GUSEK and solved with Gurobi.

3.2 Results and analysis for economic objective model

The economic objective model is developed to determine the economic feasibility and optimal capacities and locations of the distributed preprocessing facilities and integrated facilities in Minnesota by maximizing the net present profit for a 20-year project. **Figure 3a shows the forest residue availability.** The northern Minnesota has the most abundant forest residue sources, especially in Lake, Itasca, St. Louis, Koochiching, Cass, Aitkin, Hubbard, Clearwater, and Beltrami Counties. The forest residue in those nine counties

represents 70% of the total forest residue in Minnesota. Among these counties, St. Louis County has the largest amount of forest residue, representing approximately 19% of the total forest residue in Minnesota. The optimal locations for the distributed preprocessing, integrated facilities, and natural gas suppliers locations are illustrated in Figure 3b. The results predict that three integrated facilities (include the preprocess facility and biorefinery facility) and five distributed preprocessing facilities would be built in the state of Minnesota.

{Insert Figure 3 here}

~~Based on the optimization model, In St. Louis County and Cass County,~~ two of the integrated facilities with the highest capacity level (L5, 2000 metric ton/day) ~~are~~ ~~modeled~~ ~~should be~~ ~~to be built~~ ~~in St. Louis County and Cass County.~~ Although Dakota County contains only 6% of the forest residue in Minnesota, it is located very near Minneapolis-St Paul and thus ~~reduces~~ ~~reduces significant amount of the~~ transportation costs ~~significantly.~~ ~~So~~ ~~Therefore based on the model,~~ an integrated facility is ~~modeled to be~~ ~~built~~ in Dakota with capacity L4 (1000 metric ton/day). The five distributed preprocessing facilities are ~~modeled to be built~~ in Aitkin (L3), Beltrami (L4), Itasca (L3), Koochiching (L3), and Lake (L3) Counties. These facilities are ~~modeled to be built~~ in the counties rich in forest residue for convenient collection of biomass. The biomass mass flows for the distributed preprocessing facilities and their locations are shown in ~~Table~~ 1.

{Insert Table 1 here}

The main biomass mass flows to the three integrated facilities (integrated preprocessing and biorefinery) are shown in **Table 2**. Most of the biomass arriving at the St. Louis County or Cass County integrated preprocessing facilities is raw biomass or preprocessed biomass from distributed preprocessing facilities. The third integrated facility, located in Dakota County, receives raw biomass and road chipped biomass from near biomass harvest sites and preprocessing biomass from Aitkin County. The raw biomass is preprocessed and converted to commodity chemicals at this integrated facility. Each integrated facility has a natural gas supplier nearby.

{Insert Table 2 here}

A breakdown of the total cost is shown in Figure 4. The facility capital cost is the largest expenditure, representing 33% of the total cost. The production cost accounts for 30% of the total cost, which includes the fixed operating cost (19.4%) and the variable operating cost (10.3%). The remainder of the cost comes from the biomass collection and transportation cost, which are 18.9% and 18%, respectively. The transportation cost includes the costs of transporting the biomass, commodity chemicals, and the natural gas. The biomass transportation is the largest among them, representing 13.9% of the total cost.

{Insert Figure 4 here}

3.3 Factors influencing project profitability

Figure 3 describe the effect of variable factors on the project profitability. The commodity chemicals demand is directly related to project revenues. **Figure 3(a)** shows

the effect of chemicals demand on project profitability. Here the relative chemicals demand in x-axis represents ratio of chemical demand to baseline demand. The profitability increases directly with increasing chemicals demand from 25% to 75% of the current production. Profitability increases to \$494 million when chemicals demand reaches 75% of the baseline. After that, profitability stays constant even as the chemicals demand increases. This is because the forest residue is not sufficient to achieve the largest profitability possible when the chemicals demand is 75% of the baseline. So even when the chemicals demand increases, the biomass supply is not sufficient to meet the demand.

{ Insert Figure 3 here }

Based on the analysis of effect of chemicals demand variation on total profitability, it is illustrated that the biomass availability plays a significant role in the total profitability. Seasonal and other factors (competition of biomass etc.) cause variation in biomass availability and thus lead to different optimal solutions. Figure 3(b) illustrates the effect of variation of biomass availability on the project profitability. Here the relative biomass availability in the x-axis means ratio of biomass availability to baseline availability. The project profitability increases as the biomass availability increases. As discussed, the project profitability is limited by insufficient biomass. When there is an increase in biomass availability, the project profitability will increase significantly.

The competition for this feedstock will lead to increasing forest residue price. Biomass collection cost is an important parameter for the project profitability, representing 18.9%

of the total capital cost. The effect of variation in biomass collection cost on project profitability is analyzed in **Figure 3(c)**. Here the relative biomass collection cost in x-axis is ratio of biomass of collection cost with respect to the baseline biomass collection cost. It is illustrated that when the biomass collection cost is reduced to 25% of the baseline, the maximum profitability for the project increases to \$812 million. The profitability decreases to just \$165 million when the biomass collection cost is twice the baseline cost.

Facility capital cost is the largest contributor to project profitability. As indicated in **Figure 3(d)**, if the facility cost is double the baseline, there is project profitability will drop to zero. Here the relative facility capital cost in x-axis is ratio of facility capital cost with respect to the baseline.

3.4 Results and analysis for the economic-environmental multi-objective model

The multi-objective model is formulated **to** analyze the trade-off between minimizing GHG emissions and while maximizing project profits. The ϵ -constraint method is used to solve this multi-objective problem. The Pareto curve generated by all of the optimal solutions is shown in **Figure 4**. The GHG emissions reduce from 843 million kg CO₂eq per year to zero while the total 20-year profitability decreases from 494 million dollars to zero.

{Insert Figure 4 here}

In the Pareto curve, there is one integrated facility with capability L4 (1000 metric ton/day) in St. Louise for Point A. For point B, two distributed preprocessed facilities

with capacity L3 are modeled to be built in Koochiching and Lake. One integrated facility is modeled to be built with capacity of L5 level (2000 metric ton/day) in St. Louis. The emissions for Point B are 331 million kg CO₂eq /year and the profitability is \$300 million. From point A to point B, the optimal solution includes only one integrated facility (built in St. Louis County). After point B, other integrated facilities are molded to be built in addition to the integrated facility in St. Louis County. For points C, two integrated facilities are molded to be built which are located in St. Louis (L5, 2000 metric ton/day) and Beltrami (L4, 1000 metric ton/day) and the distributed preprocessing facilities are molded to be built in Itasca, Lake and Koochiching. Point D is a good point where two integrated facilities and five distributed preprocessing facilities are molded to be built. The two integrated facilities are located in St. Louis (L5, 2000 metric ton/day) and Case (L5, 2000 metric ton/day). The five distributed preprocessing facilities are located in Itasca, Lake, Koochiching, Aitkin, and Beltrami.

The Pareto curve illustrates the trade-offs between economics and environmental effects. When the production capacity is comparatively small, the profitability grows fast with a small increase of GHG emissions. After a certain production capacity (point B), however, the profitability grows much slowly. From point A to point D, the optimal integrated facility locations always include St. Louis County, which indicates that St. Louis County is the most favorable location to build the integrated chemicals plant.

4. Conclusions

This work investigates the economic feasibility and the optimal production planning and facility locations for commodity chemicals production via woody biomass fast pyrolysis. The economic objective model results show that the distributed facilities biomass chipping is preferable to the roadside chipping method for forest residue. The harvest sites rich in biomass resources are the preferable locations for building biorefinery facilities. Influences of parameters on economic objective model show that the biomass availability and facility capital costs are the most important factors for the project profitability. The economic-environmental multi-objective model results illustrate the trade-off between economic and environmental considerations.

Acknowledgements

The authors would like to acknowledge the financial support of the Bioeconomy Institute and the Biobased Industry Center of Iowa State University and the National Science Foundation under Grant Number EPS-1101284.

References

1. An, H., Wilhelm, W.E., Searcy, S.W. 2011. A mathematical model to design a lignocellulosic biofuel supply chain system with a case study based on a region in Central Texas. *Bioresource Technology*, 102(17), 7860-7870.
2. Bai, Y., Hwang, T., Kang, S., Ouyang, Y. 2011. Biofuel refinery location and supply chain planning under traffic congestion. *Transportation Research Part B: Methodological*, 45(1), 162-175.

3. Blottnitz, H.v., Curran, M.A. 2007. A review of assessments conducted on bio-ethanol as a transportation fuel from a net energy, greenhouse gas, and environmental life cycle perspective. *Journal of Cleaner Production*, 15(7), 607-619.
4. Bowling, I.M., Ponce-Ortega, J.M.a., El-Halwagi, M.M. 2011. Facility Location and Supply Chain Optimization for a Biorefinery. *Industrial & Engineering Chemistry Research*, 50(10), 6276-6286.
5. Brehmer, B., Boom, R.M., Sanders, J. 2009. Maximum fossil fuel feedstock replacement potential of petrochemicals via biorefineries. *Chemical Engineering Research and Design*, 87(9), 1103-1119.
6. Brown, T.R., Zhang, Y., Hu, G., Brown, R.C. 2012. Techno-economic analysis of biobased chemicals production via integrated catalytic processing. *Biofuels, Bioproducts and Biorefining*, 6(1), 73-87.
7. BTS. 2012. Average Freight Revenue per Ton-mile. Bureau of Transportation Statistics. (Available at: http://www.bts.gov/publications/national_transportation_statistics/html/table_03_21.html (accessed November, 2012))
8. BTS. 2007. Commodity Flow Survey 2007. Table 12. Shipment Characteristics by NAICS and Commodity for Metropolitan Area of Origin: 2007. Available at: http://www.rita.dot.gov/bts/sites/rita.dot.gov.bts/files/publications/commodity_flow_survey/2007/metropolitan_areas/minneapolis_st_paul_st_cloud_mn_wi_csa_mn_part/index.html
9. CBO. 1982. Energy use in freight transportation. *Congressional Budget Office*.

10. Christensen, C.H., Rass-Hansen, J., Marsden, C.C., Taarning, E., Egeblad, K. 2008. The Renewable Chemicals Industry. *ChemSusChem*, 1(4), 283-289.
11. Dale, B.E. 2003. 'Greening' the chemical industry: research and development priorities for biobased industrial products. *Journal of Chemical Technology & Biotechnology*, 78(40), 1093-1103.
12. Dunnett, A., Adjiman, C., Shah, N. 2008. A spatially explicit whole-system model of the lignocellulosic bioethanol supply chain: an assessment of decentralised processing potential. *Biotechnology for Biofuels*, 1(4), 1-17.
13. EIA. 2011. Natural Gas Annual Respondent Query System. (Available at: http://www.eia.gov/cfapps/ngqs/ngqs.cfm?f_report=RP7)
14. Elia, J.A., Baliban, R.C., Floudas, C.A., Gurau, B., Weingarten, M.B., Klotz, S.D. 2013. Hardwood Biomass to Gasoline, Diesel, and Jet Fuel: 2. Supply Chain Optimization Framework for a Network of Thermochemical Refineries. *Energy & Fuels*, 27, 4325-4352.
15. Gavrilescu, M., Chisti, Y. 2005. Biotechnology—a sustainable alternative for chemical industry. *Biotechnology Advances*, 23(7-8), 471-499.
16. Giarola, S., Shah, N., Bezzo, F. 2012. A comprehensive approach to the design of ethanol supply chains including carbon trading effects. *Bioresource Technology*, 107(4), 175-185.
17. Hamelinck, C.N., Hooijdonk, G.v., Faaij, A.P.C. 2005. Ethanol from lignocellulosic biomass: techno-economic performance in short-, middle- and long-term. *Biomass and Bioenergy*, 28(4), 384-410.

18. Hess, J.R., Wright, C.T., Kenney, K.L. 2007. Cellulosic biomass feedstocks and logistics for ethanol production. *Biofuels, Bioproducts and Biorefining*, 1(3), 181-190.
19. Kim, J., Realff, M.J., Lee, J.H. 2011. Optimal design and global sensitivity analysis of biomass supply chain networks for biofuels under uncertainty. *Computers & Chemical Engineering*, 35(9), 1738-1751.
20. Oak Ridge National Laboratory (ORNL) 2007. Survey of Alternative Feedstocks for Commodity Chemical Manufacturing. (Available at: http://cepac.cheme.cmu.edu/pasi2011/library/cremaschi/Survey_of_alternative_feedstocks_for_the_chemical_industry.pdf)
21. Larson, E.D. 2006. A review of life-cycle analysis studies on liquid biofuel systems for the transport sector. *Energy for Sustainable Development*, 10(2), 109-126.
22. Leinonen, A. 2004. Harvesting Technology of Forest residues for fuel in the USA and Finland. (Available at: <http://www.vtt.fi/inf/pdf/tiedotteet/2004/T2229.pdf>)
23. NREL. 2013. Forest and Primary Mill Residues, 2013. (Available at: http://www.nrel.gov/gis/data_biomass.html)
24. Rogers, J.G., Brammer, J.G. 2009. Analysis of transport costs for energy crops for use in biomass pyrolysis plant networks. *Biomass and Bioenergy*, 33(10), 1367-1375.
25. Schilling, L.B. 1995. Chemicals from alternative feedstocks in the United States. *FEMS Microbiology Reviews*, 16(2-3), 101-110.

26. Searcy, E., Flynn, P., Ghafoori, E., Kumar, A. 2007. The relative cost of biomass energy transport. *Applied Biochemistry and Biotechnology*, 137-140(1-12), 639-652.
27. Stephen, J.D., Mabee, W.E., Saddler, J.N. 2010. Biomass logistics as a determinant of second-generation biofuel facility scale, location and technology selection. *Biofuels, Bioproducts and Biorefining*, 4(5), 503-518.
28. Tallaksen, J. 2011. Biomass Gasification: A Comprehensive Demonstration of a Community Scale Biomass Energy System. **Final Report, USDA Rural Development, Grant 68-3A75-5-232.**(Available at: http://renewables.morris.umn.edu/biomass/documents/USDA_Report/USDA_Main_Report.pdf)
29. Vispute, T.P., Zhang, H., Sanna, A., Xiao, R., Huber, G.W. 2010. Renewable Chemical Commodity Feedstocks from Integrated Catalytic Processing of Pyrolysis Oils. *Science*, 330(6008), 1222-1227.
30. You, F., Tao, L., Graziano, D.J., Snyder, S.W. 2012. Optimal design of sustainable cellulosic biofuel supply chains: Multiobjective optimization coupled with life cycle assessment and input–output analysis. *AIChE Journal*, 58(4), 1157-1180.
31. You, F., Wang, B. 2011. Life Cycle Optimization of Biomass-to-Liquid Supply Chains with Distributed–Centralized Processing Networks. *Industrial & Engineering Chemistry Research*, 50(17), 10102-10127.

32. Zhang, Y., Brown, T.R., Hu, G., Brown, R.C. 2013a. Comparative techno-economic analysis of biohydrogen production via bio-oil gasification and bio-oil reforming. *Biomass and Bioenergy*, 51(9), 99-108.
33. Zhang, Y., Brown, T.R., Hu, G., Brown, R.C. 2013b. Techno-economic analysis of two bio-oil upgrading pathways. *Chemical Engineering Journal*, 225(9), 895-904.
34. Zhang, Y., Hu, G., Brown, R.C. 2013c. Life cycle assessment of commodity chemicals production from forest residue via fast pyrolysis. Technical Report, Iowa State University.
35. Zhang, Y., Hu, G., Brown, R.C. 2013d. Life cycle assessment of the production of hydrogen and transportation fuels from corn stover via fast pyrolysis. *Environmental Research Letters*, 8(2), 025001.

Figure captions

Figure 1. Process diagram for mixed wood fast pyrolysis and bio-oil upgrading to commodity chemicals (Adapted from Zhang et al. (2013(b))).

Figure 2. Supply chain schematic for chemicals production via woody biomass fast pyrolysis.

Note: This figure is a schematic diagram of the biomass flows; it does not represent an actual number of facilities.

Figure 3. Effects of chemicals demand, biomass availability, biomass collection cost and facility capital cost on project profitability.

Figure 4. Pareto curve for the economic-environmental multi-objective optimization for supply chain of commodity chemicals production via woody biomass fast pyrolysis.