AIChE

Nationwide Energy Supply Chain Analysis for Hybrid Feedstock Processes with Significant CO_2 Emissions Reduction

Josephine A. Elia, Richard C. Baliban, and Christodoulos A. Floudas
Dept. of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544

DOI 10.1002/aic.13842
Published online May 29, 2012 in Wiley Online Library (wileyonlinelibrary.com).

Integrating diverse energy sources to produce cost-competitive fuels requires efficient resource management. An optimization framework is proposed for a nationwide energy supply chain network using hybrid coal, biomass, and natural gas to liquids (CBGTL) facilities, which are individually optimized with simultaneous heat, power, and water integration using 162 distinct combinations of feedstock types, capacities, and carbon conversion levels. The model integrates the upstream and downstream operations of the facilities, incorporating the delivery of feedstocks, fuel products, electricity supply, water, and CO_2 sequestration, with their geographical distributions. Quantitative economic trade-offs are established between supply chain configurations that (a) replace petroleum-based fuels by 100%, 75%, and 50% and (b) utilize the current energy infrastructures. Results suggest that cost-competitive fuels for the US transportation sector can be produced using domestically available coal, natural gas, and sustainably harvested biomass via an optimal network of CBGTL plants with significant GHG emissions reduction from petroleum-based processes. *AIChE J*, 58: 2142–2154, 2012
Keywords: optimization, energy, mathematical modeling, supply chain, transportation fuels

Introduction

In an era of intensifying oil resource constraints, hybrid feedstock energy processes are an attractive avenue towards a more sustainable energy future due to their flexibility in converting multiple types of inputs into a consistent range of products. The commercially deployable Fischer-Tropsch technology forms a platform of such hybrid energy processes, as it can convert synthesis gas from coal, biomass, natural gas, or a combination of these feedstocks into synthetic fuels that supplement or replace petroleum-derived fuels, potentially moving the United States away from oil imports to domestic resources.[1–12]

Recently, a novel example that illustrates the versatility of hybrid energy processes is demonstrated in a coal, biomass, and natural gas to liquids (CBGTL) process that produces gasoline, diesel, and kerosene in proper ratios for the United States demands.[2,13–18] (Baliban, et al., 2012, submitted) Among the unique components of the initial design is the recycle of CO_2 into the process via the reverse water gas shift reaction. The proposed process is expanded into a thermochemical CBGTL superstructure that includes multiple pathways to convert coal, biomass, and natural gas to transportation fuels, including (i) alternative process units for fuel conversion, (ii) stream interconnectivities between process units, and (iii) multiple unit operating conditions. An optimization-based framework is developed to identify the most profitable plant topology with simultaneous heat, power, and water integration to minimize utility consumption for the process, and an environmental constraint is included in the model such that the life cycle greenhouse gas (GHG) emissions achieves at least 50% reduction from petroleum-based processes. This emissions target is achieved through a combination of biomass utilization, which takes carbon from the atmosphere during cultivation, CO_2 sequestration, and CO_2 recycle into the process. A global optimization framework has been proposed to achieve the optimal plant design with theoretical guarantee that the cost is within a small percentage of the lowest possible cost.[18] The proposed optimization framework that considers a superset of technologies for liquid fuel conversion yields a plant topology that is both economically viable and environmentally beneficial.

In a supply chain analysis for such hybrid processes, the integration of multiple sources necessitates the cooperation of several economic domains to achieve efficient resource allocation and a cost-competitive supply chain.[15,19,20] For example, as a mitigating factor for GHG emissions, biomass must be sustainably harvested using idle agricultural land that will not adversely affect the food supplies.[21,22] Such sustainable biomass includes agricultural and forest residues, and perennial grasses grown on uncultivated land under the United States Department of Agriculture's Conservation Reserve Program (CRP).[12,15] These biofeedstock producing areas are dispersed across the country and stand in contrast with coal and natural gas producing areas, which are centralized in fewer locations. This contrast elicits an important question on how to optimally locate the hybrid energy facilities and to allocate these resources efficiently. In addition to the carbon feedstocks, considerations of other factors such as

Additional Supporting Information may be found in the online version of this article.

Correspondence concerning this article should be addressed to C. A. Floudas at floudas@titan.princeton.edu.

electricity and freshwater consumption, and the management of the vented or sequestered CO_2 have to be taken into account. Thus, an integrated and systematic approach that can elucidate the interdependence between key stakeholders at once and attain a synergistic effect between these different sectors is necessary. Although energy supply chain problems are present in literature,[23–29] a comprehensive approach that takes the scope at the nationwide level has not been undertaken.

In this article, we propose an optimization framework to address a large-scale, nationwide CBGTL supply chain problem that accounts for the varying configurations of feedstock productions and the demand profile for transportation fuels in the United States. The CBGTL supply chain builds on the framework applied to the single CBGTL plant by Baliban et al.[16–18] (Baliban, et al., 2012, submitted) that optimizes the plant topology with simultaneous heat, power, and water integration. The supply chain begins at the feedstock locations, ends at the demand locations, and is optimized to yield the strategic placements of CBGTL facilities across the country with minimum overall cost of fuel production, attaining competitive products and significantly less environmental impacts compared to petroleum processes. The supply chain also addresses the electricity supply, water supply, and the allocation of sequestered CO_2 to injection sites. The total liquid fuels produced by the entire supply chain network meet the demand for the United States, and the formulated large-scale mixed-integer linear optimization (MILP) model for the problem includes representations of the discrete decisions (e.g., where to locate the CBGTL plants, what type of plant should be built) and continuous decisions (e.g., the interconnections between feedstock sources, facility locations, and demand locations, the flow rate amount for each connection) that need to be made to satisfy the fuel demands with competitive economic and environmental performances. These facets of the solution provide a quantitative basis to examine the trade-offs of investment decisions for the hybrid energy supply chain.

The unique features of this work are: (i) the incorporation of a process synthesis framework for individual plant design that includes onsite hydrogen production, methanol synthesis and conversion to gasoline, and ZSM5 upgrading of liquid fuels,[18] (Baliban, et al., 2012, submitted) (ii) simultaneous heat, power, and water integration in the plant design, (iii) hybrid CBGTL plants with multiple carbon conversion levels, (iv) CO_2 management via a combination of sequestration, recycle, and venting, (v) incorporation of the distribution and injection sites for sequestered CO_2 in the supply chain, (vi) incorporation of renewable electricity generation in the supply chain and an imposed maximum of grid electricity expansion, (vii) incorporation of freshwater supply chain, (viii) finer granularity in the candidate facility locations, and (ix) life cycle analysis on a single plant basis and on the entire supply chain network.

Model Parameter Inputs

To address the aforementioned issues and to identify an efficient nationwide hybrid energy supply chain network, parameter inputs and supporting data are necessary for the optimization problem. The specific inputs to the mathematical model include (i) the locations, availabilities, and purchase costs of coal, biomass, and natural gas feedstocks, (ii) the locations and amounts of liquid fuel demands, (iii) the locations, availabilities, and costs of electricity, water, and CO_2 sequestration sites, (iv) the parameters associated with the investment costs and operation of CBGTL facilities (i.e., input and output flow rates of materials to and from the facilities), (v) the configuration of the CBGTL candidate facility locations, and (vi) the modes of transportation to deliver various materials considered in the problem.

To fulfill the fuel demands of the entire United States, multiple combinations of coal and biomass feedstocks that are available domestically need to be considered. The carbon feedstock parameters, which include the location, availabilities, and purchase prices of coal, biomass, and natural gas, are obtained from published government-based databases and follow the methods outlined in Elia et al. (2011).[15] Six coal types (i.e., lignite, sub-bituminous, high-, medium-, and low-volatile (HV, MV, LV) bituminous, and anthracite coal) are included in the supply chain analysis.[15] In this article, however, biomass is categorized into three representative groups, namely the forest residues, the agricultural residues, and the perennial grasses.[30] This categorization is based on Elia et al. (2011),[15] which includes nine species for agricultural residues, five species for forest residues, and one for perennial grasses, and the feedstock parameters for the biomass species are grouped into their corresponding categories. Finally, one generic composition for natural gas is used based on an average composition of natural gas wellhead productions in the United States.[31] Based on the available databases, coal and biomass sources, as well as their prices, are discretized on a county basis, and natural gas sources are discretized on a state basis. Note that the spatial variations on both the availabilities and purchase prices of each feedstock are taken into account in the mathematical model.

Similarly, the fuel demand parameters (i.e., the demand locations of gasoline, diesel, and kerosene in the United States, and their corresponding amounts) and the modes of transportation considered in the energy supply chain (i.e., railway for coal, truck for biomass, interstate and intrastate pipelines for natural gas, and a combination of barges, truck, and pipelines for liquid fuel products), as well as a new set of CBGTL plant parameters, candidate locations, parameters for electricity, water, and CO_2 management are introduced and described in the sequel.

CBGTL plant parameters

As each CBGTL plant is designed to receive only one type of coal, biomass, and natural gas composition into the process, a variety of plant topologies that take distinct combinations of coal and biomass feedstocks needs to be generated.[16–18] (Baliban, et al., 2012, submitted) Using the approach outlined by Baliban et al.,[16,17] (Baliban, et al., 2012, submitted) a total of 162 distinct topologies, combining six coal feedstock types, three representative biomass types, one natural gas composition, three plant capacities (i.e., 10,000 barrels per day (BPD), 50,000 BPD, and 200,000 BPD), and three feedstock-to-fuel carbon conversion levels (i.e., 40, 50, and 60%) can exist in the supply chain network. The capacities of the CBGTL facilities are selected based on the current refinery capacities in the United States, which range from 2,000 to 572,500 barrels per day.[15] The three carbon conversion levels are explicitly calculated based on the CBGTL process, which has been modeled in detail by Baliban et al.[16–18] (Baliban, et al., 2012, submitted) All process units in the syngas generation, syngas cleaning, hydrocarbon production, hydrocarbon upgrading, oxygen and hydrogen production sections are modeled mathematically, along with complete heat, power, and water integration of the whole process. The three conversion levels (i.e., 40, 50, and 60%) are selected based on a range of electricity demand/output and the amounts of feedstock that the topologies require. Conversion levels lower than 40% result in topologies that produce high amount of electricity, but require high amounts of carbon feedstocks to produce the same amount of liquid fuels. Conversely, higher conversion levels than 60% result in topologies that require less amount of feedstocks, but demand high amount of electricity input. The three selected values represent a good range of options that balance between the feedstock and electricity demand in the supply chain, as well as the combinatorial complexity of the model.

Each of the 162 distinct topologies is extracted out of a superstructure of conversion routes via a mixed-integer nonlinear optimization (MINLP) model to achieve minimum production cost with efficient heat, power, and water utilization within each plant complex.[16,17] (Baliban, et al., 2012, submitted) The superstructure used in this article is the complete superstructure that includes the methanol-to-gasoline conversion process and the upgrading of liquid fuels over zeolite catalyst (ZSM5) detailed by Baliban et al. (2012, submitted). The simultaneous heat and power integration is done by introducing heat engines that interact with process streams to recover waste heat and produce steam and electricity for the process.[14,16,17] The minimization of freshwater consumption and wastewater effluent is done by including a comprehensive water network that includes a sour stripper and a biological digester to remove acidic gases and organic materials in the process water streams, and a reverse osmosis system to treat the cooling water, boiler feed water, and the steam cycles in the heat and power integration network.[17] Thus, the resulting optimal plant topology represents the best possible plant configuration with respect to the main process units and their associated utilities. Although global optimization frameworks have been developed for the process synthesis problem,[18] good quality local solutions are used in this paper for the 162 CBGTL plant topologies.

The three plant capacities that may exist in the supply chain are selected not only to allow for economies of scale with increased capacities, but also to take into account the variability of feedstock availabilities in different regions. Although candidate locations close to abundant coal, biomass, and natural gas resources may favor the selection of larger facilities, other more remote areas may still produce liquid fuels locally in a smaller scale. Finally, the three carbon conversion levels are selected to allow trade-offs between feedstock, electricity, and water consumptions, as well as the amounts of CO_2 sequestered from the CBGTL network. For example, as the electricity usage between the three carbon conversion levels differs (i.e., most of the 40% conversion facilities produce electricity), a combination of these plants can be used to achieve a specified target of total electricity consumption/production in the country, as explained in a subsequent section of this article.

Each CBGTL plant is designed to produce gasoline, diesel, and kerosene in the same proportions as the United States transportation fuel demands,[13,16–18] (Baliban, et al., 2012, submitted) and the optimal topology of each CBGTL plant is constrained to achieve at least 50% well-to-wheel GHG emissions reduction from petroleum-based processes. In other words, the maximum well-to-wheel GHG emissions from the CBGTL process is equal to half of the well-to-wheel emissions of petroleum based processes. The average emissions of petroleum fuels have been calculated to be 91.6 kg CO_2 equivalent/GJ lower heating value (LHV) of fuels produced,[6] and the new limit for the CBGTL processes is equal to 45.8 kg CO_2 equivalent/GJ LHV. Although multi-objective optimization approaches are present in literature to include both economic and environmental objectives,[32] the environmental performance in this work is represented as a constraint. This emissions reduction target of $\sim$ 50% from petroleum emissions represents the 2050 target agreed by global leaders at the G8 Summit.[33] The process synthesis optimization model directly accounts for the well-to-wheel life cycle emissions calculation that starts from the GHG emitted during feedstock acquisition, feedstock transportation, the CBGTL process, fuel product delivery, and ends with the consumption of liquid fuels. Biomass provides a negative balance to the emissions figure and can be used to achieve the emissions target, combined with CO_2 sequestration and recycle into the process. A maximum of 15% of the input carbon can be emitted from the CBGTL plant to the atmosphere, and the rest is either sequestered or recycled back into the CBGTL process. The CBGTL process is able to react recycled CO_2 with input H_2 to yield CO and H_2O via the reverse water gas shift reaction in the coal and biomass gasifiers, Fischer-Tropsch reactors, or a dedicated reverse water gas shift reactor.[16,17] (Baliban, et al., 2012, submitted) A detailed method for the life cycle analysis (LCA) is included in a subsequent section. The 162 optimized plant topologies represent the facility types that the energy supply chain optimization model can select for any given candidate location, and the process synthesis framework ensures that the topologies are both economically viable and environmentally advantageous for the transportation sector. Detailed results from the 162 optimization runs are included in Supporting Information Tables S1–S6.

Candidate facility locations

The configuration for the candidate facility location is based on a postulated superset of county-based candidate locations for the contiguous 48 states. For a county to be a valid candidate location, it must be able to receive coal, biomass, and natural gas from the surrounding areas, given that its transportation cost is within the upper bounds imposed to prevent unrealistically large distances traveled by each feedstock. Biomass is transported by truck, coal is transported by rail, and natural gas is transported via interstate and intrastate pipelines. All valid locations are then ranked separately based on the availabilities of coal, biomass, and natural gas in each county, and the combined rank order list provides the basis of eliminating less favorable sites. The top 70% sites per state are selected as valid candidate locations based on a parametric analysis that demonstrates the trade-offs between improved values of the objective function, increased computational time, and model complexity. The reduced set consists of 1,329 candidate locations for the CBGTL supply chain network. A detailed description of the approach for the generation of this set is included in Appendix A.

Electricity

The electricity usage from the CBGTL facilities adds to the electrical power demand for the country. In the United

States, the net electricity generation capacity in 2009 is reported to be 1025.4 GW in the summer and 1063.8 GW in the winter.[34] Because most of the country's electrical power still relies currently on fossil fuels, it is important to cap the total electricity usage in the supply chain network to prevent excessive expansion of the current power supply. This goal is achieved in two ways in this article, namely (i) on a single plant approach, and (ii) on a network based approach. From the design of single plants, the selection of three carbon conversion levels provides the supply chain network with a combination of plants that are net consumers and net producers of electricity. On a network based approach, a total cap is imposed on the grid expansion for the whole country, which is set to be at most 10% of current generation, amounting to a total of 102.5 GW.

Additionally, the electrical power generated from renewable sources is incorporated into the supply chain. When a plant produces electricity, it can be placed anywhere in the country and a profit will be taken from selling electricity to the grid. However, when a plant requires electricity, three options are available, namely drawing electricity from the grid, producing electricity from solar resources, or producing electricity from wind resources. The investment costs of each electricity option are accounted in the model, and the optimization model will select one or a combination of electricity sources for a given selected facility.

Electricity from solar and wind is assumed to be produced from solar and/or wind plants built onsite. The maximum capacity is set to 40 MW for a wind plant and 20 MW for a solar plant. Only candidate locations that have adequate solar irradiation and wind speed are allowed to include solar and wind plants. Solar irradiation data are obtained from the National Solar Radiation Data Base (NSRDB) 1991–2005 Update.[35] The longitude and latitude data of the station sites where solar irradiation data are defined are used to calculate the distance between solar sites and candidate locations of CBGTL plants. If a candidate location for a CBGTL facility is within 10 miles of a solar station site, and the data indicate that there is adequate irradiation surrounding the candidate location, then a solar plant may be built onsite, where the CBGTL facility is built.

Wind profiles across the United States are obtained from the National Renewable Energy Laboratory (NREL) Wind Integration Dataset,[36] namely the Eastern Wind Dataset and the Western Wind Datasets. The Western Wind Datasets contain 32,043 locations with the highest wind energy density in the western part of the United States. From the Eastern Wind Datasets, sites from the land based and Midwest ISO (MISO) areas are used in this analysis. The longitude and latitude data of the station sites are used to calculate the distance between wind sites and candidate locations of CBGTL plants. If a candidate location for a CBGTL facility is within 10 miles of a wind site, and the data indicate that there is adequate wind speed surrounding the candidate location, then a wind farm may be built onsite, where the CBGTL facility is built. The investment costs of building these facilities are taken into account, and as they are assumed to be built onsite, the need and costs for transmission and electrical grid expansion are eliminated.

Water resources

The freshwater input to the CBGTL facilities will add to the national freshwater consumption figure, putting additional stress on water resources. In energy processes, water is typically used for washing operations, separation processes, steam and power generation, cooling systems, or as a raw material input to the processes, and the discharged wastewater needs to be treated before the final disposal to the environment and the treatment processes can be energy intensive.[37,38] To prevent massive consumption of water for the CBGTL plants, strategies are implemented on both the single plant and network-based approaches. The water superstructure incorporated in the process synthesis framework ensures that the freshwater input and wastewater discharge of the CBGTL plants are minimized, thus minimizing the stress on water resources.

As the stress on water resources varies from region to region, it is important to consider the availability of water resources in the placement of new CBGTL plants. Thus, the water supply to CBGTL facilities is incorporated to the energy supply chain model. Data on the use of water in the United States are obtained from the United States Geological Survey (USGS) database.[39] For each county, estimates of freshwater consumption for domestic, agricultural, and industrial sectors are reported. The water availability is calculated by taking the minimum of 1.5 times of current industrial use or 15% of total freshwater use in the county. All connections from water resource locations and the facility locations are postulated, and the water requirement of an existing plant must be supplied by locations within 200 miles its radius to ensure that local resources are utilized.

CO_2 sequestration

As the CBGTL plants require CO_2 sequestration, it is important to ask the questions of where would the sequestration sites be located in the United States and what are their capacities, since they can affect the locations of CBGTL facilities. As potential geological storage sites are being explored, only estimates are currently available on the capacities of CO_2 sequestration. The estimates from the National Energy Technology Laboratory (NETL)[40] Atlas project are used in this study to determine the locations and capacities of CO_2 storage. Appendix C of the document[40] is used to calculate the total estimated storage resources (high capacity scenario) by state and the locations of the sites are assumed to be at the center of the state. Note that the approach taken in the optimization model can be readily used where more discretized information on storage sites become available.

The sequestered CO_2 exits the CBGTL plant at 150 bar and is transported via pipeline to the storage sites. The levelized costs of investment for CO_2 pipelines are calculated using a piecewise linearization of the pipeline equations in Ogden (2004)[41] as functions of the CO_2 flow rates and transportation distances, which are calculated explicitly in the model. The cost of injection and levelized cost for new wells also follow the approach in Ogden (2004)[41] and are minimized in the energy supply chain optimization model. The amounts of CO_2 sequestered and vented from the 162 plant topologies can be found in Supporting Information Tables S4–S6.

Life cycle analysis

GHG emissions throughout the life cycle of the CBGTL process are calculated to maintain a target of at least 50% reduction from petroleum-based fuels. The contributing segments to the overall emissions figure include emissions from

(i) biomass, coal, and natural gas acquisitions, (ii) transportation of feedstock from their source locations to the CBGTL facilities, (iii) carbon storage in the biomass feedstock, (iv) carbon storage in the soil and root during biomass cultivation for perennial grasses, (v) vented CO_2 from the CBGTL process, (vi) electricity production, (vii) transportation of fuel products, and (viii) consumption of fuel products. A complete calculation method for the life cycle analysis can be found in Elia et al. (2011).[15]

A notable factor in the life cycle analysis (LCA) is the biomass feedstock that provides emissions credit due to the carbon accumulation via photosynthesis during its cultivation. Perennial grasses are assumed to grow on degraded, carbon-deficient soil, so an additional carbon soil storage benefit of 31.3% kg carbon/kg dry biomass can be claimed from the land use change.[7] The LCA calculation for each CBGTL facility is completed in both the single plant design level and on the network based level. First, the process synthesis approach contains a LCA constraint of at most 50% of petroleum-based processes (i.e., 45.8 kg $CO_{2,eq}$/GJ fuels) that also determines the amount of biomass input flow rate into the system. At this stage, the distances traveled for feedstock and fuel transportations are assumed from distances for internodal transportation obtained from the GREET model.[15,42] Note that the LCA constraint in the process synthesis model does not include emissions due to electricity, because electricity can be taken from the grid and renewable sources in the supply chain. If electricity from the grid is selected, than an additional emissions factor is added to the LCA, but if renewable electricity is selected, no additional emissions are added to the LCA. In the supply chain optimization model, assumptions on the distance traveled are removed since they can be explicitly calculated in the model, giving the most accurate accounting of the emissions level, and each selected CBGTL plant has an associated emissions figure. The emissions due to electricity generation are then added to the final LCA.

Energy Supply Chain Optimization Model

The 162 CBGTL plant designs along with nationwide coal, biomass, and natural gas feedstock productions, fuel demands, electricity supply, water resources, CO_2 sequestration capacities, the modes of transportation for each material flow, and a configuration of candidate facility locations, become the parameter inputs into the energy supply chain optimization model. The energy supply chain optimization problem is formulated as a large-scale MILP model, solved to give the optimal network layout of the CBGTL supply chain at the minimum overall cost of fuel production for the entire network. The model yields (i) the strategic locations of CBGTL facilities throughout the country, (ii) the specific types and capacities of the selected facilities, (iii) the complete supply chain topology from the feedstock sources to the demand locations with the flow rate amounts of each interconnection, and (iv) the costs associated with each segment of the supply chain problem. The complete formulation and description of the mathematical model are as follows.

Continuous variables are used to represent the levelized investment cost at a particular location (Cost_l^I), the total electricity requirement (El_l^T), electricity produced (El_l^P), solar electricity required (El_l^S), wind electricity required (El_l^W), grid electricity required (El_l^G), the water requirement (WF_l), the CO_2 sequestration amount (SF_l), the flow of feedstock from the producing locations to the plant facility ($x_{f,c,l,m}$), the required flow rate of feedstocks to a plant facility ($FR_{f,l}$), the flow of products transported from the plant facility to the demand locations ($z_{p,l,c,m}$), the flow of freshwater to the facilities ($w_{c,l}$), and the sequestration amount from a facility ($\mathrm{seq}_{c,l}$). Binary variables ($y_{f,f',f'',l,t,q}$) represent the selection of a specific CBGTL plant type at location l with feed combination $(f,f',f'') \in FC$, size t, and carbon conversion option q. The complete variable list can be found in the Notation Section.

Equation 1 restricts the selection of CBGTL facilities such that at most one facility can be selected at a given candidate location. Equations 2–4 impose lower and upper limits in the number of selected CBGTL facilities for the entire network, both overall and per plant capacity. Typical bounds used in this article are $N = 500$, $N_t^{\max} = 300\ \forall t$, and $N_t^{\min} = 0\ \forall t$.

$$\sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',t,l,q} \le 1 \quad \forall l \in L^F \tag{1}$$

$$\sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',l,t,q} \le N \tag{2}$$

$$\sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',l,t,q} \le N_t^{\max} \quad \forall t \in T \tag{3}$$

$$\sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',l,t,q} \ge N_t^{\min} \quad \forall t \in T \tag{4}$$

Selection of the investment cost parameters and the feedstock requirements associated with active facilities is determined by Equations 5–8.

$$\sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',l,t,q} LC_{f,f',f'',t,q} = \mathrm{Cost}_l^I \quad \forall l \in L^F \tag{5}$$

$$FR_{f,l} = \sum_{(f,f',f'',t,l,q)\in FL} FR^C_{f,f',f'',t,q} y_{f,f',f'',l,t,q} \quad \forall f \in F^C, l \in L^F \tag{6}$$

$$FR_{f',l} = \sum_{(f,f',f'',t,l,q)\in FL} FR^B_{f,f',f'',t,q} y_{f,f',f'',l,t,q} \quad \forall f' \in F^B, l \in L^F \tag{7}$$

$$FR_{f'',l} = \sum_{(f,f',f'',t,l,q)\in FL} FR^G_{f,f',f'',t,q} y_{f,f',f'',l,t,q} \quad \forall f'' \in F^G, l \in L^F \tag{8}$$

Equation 9 constrains the flow rates from each feedstock source locations not to exceed the amount available at that location. Subsequently, the total flow rates arriving at a particular plant has to match the feedstock requirement of the CBGTL plant at the given location (Eq. 10). For natural gas flows, the amount transported via interstate pipelines must be within available capacities for the CBGTL supply chain network (i.e., it doesn't interfere with current usage of the pipelines; Eq. 11). Finally, Equation 12 constrains the product ratios exiting each CBGTL facility to match the United States demands for gasoline, diesel, and kerosene, and the product flow rates arriving at each demand location must meet exactly the demand amount (Eq. 13).

$$\sum_{(f,c,l,m)\in FT} x_{f,c,l,m} \leq FA_{f,c} \quad \forall (f,c) \in C_F \tag{9}$$

$$\sum_{(f,c,l,m)\in FT} x_{f,c,l,m} = FR_{f,l} \quad \forall f \in F, l \in L^F \tag{10}$$

$$\sum_{(f,c,l,m)\in FT} x_{f,c,l,m} \leq \mathrm{Cap}_m - \mathrm{Usage}_m \quad \forall m \in M^G_{\mathrm{Pipe}}, f \in F^G \tag{11}$$

$$\sum_{(p,l,c,m)\in PT} z_{p,l,c,m} = \sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',l,t,q} \mathrm{Prod}_t \mathrm{Ratio}_p \quad \forall l \in L^F, p \in P \tag{12}$$

$$\sum_{(p,c,l,m)\in PT} z_{p,l,c,m} = DM_{p,c} \quad \forall (p,c) \in C_P \tag{13}$$

The constraints associated with electricity requirement and production by the selected facilities include Equations 14–19. Produced electricity is assumed to be sold to the grid at \$0.07/kWh. Equations 14 and 15 define the electricity requirement and production for each selected facility, respectively. The electricity requirement is fulfilled in a combination of three ways, through solar, wind, or grid electricity (Eq. 16). The amount of solar and wind electricity is capped at 20 MW and 40 MW, respectively, for locations that receive enough solar irradiation and wind speed for electricity generation (Eqs. 17 and 18). Finally, a maximum for the total grid electricity expansion for the whole country is imposed (Eq. 10). In this article, Cap^G is equal to 102.5 GW (i.e., about 10% increase of the grid capacity in 2009.[34]).

$$\sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',l,t,q} EL_{f,f',f'',t,q} = El^T_l \quad \forall l \in L^F \tag{14}$$

$$\sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',l,t,q} EP_{f,f',f'',t,q} = El^P_l \quad \forall l \in L^F \tag{15}$$

$$El^T_l = El^S_l + El^W_l + El^G_l \quad \forall l \in L^F \tag{16}$$

$$El^S_l \leq \mathrm{Cap}^S_l \quad \forall l \in L^S \tag{17}$$

$$El^W_l \leq \mathrm{Cap}^W_l \quad \forall l \in L^W \tag{18}$$

$$\sum_{l\in L^F} El^G_l \leq \mathrm{Cap}^G \quad \forall l \in L^F \tag{19}$$

Equation 20 defines the freshwater input requirement for each selected facility. This value has to be matched with all water flowrates from various sources (Eq. 21) and they cannot exceed the water availabilities in each source location (Eq. 22).

$$\sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',l,t,q} FW_{f,f',f'',t,q} = WF_l \quad \forall l \in L^F \tag{20}$$

$$WF_l = \sum_{c\in C_W} w_{c,l} \quad \forall l \in L^F \tag{21}$$

$$\sum_{l\in L^F} w_{c,l} \leq WA_c \quad \forall c \in C_W \tag{22}$$

Similarly, Eq. 23 determines the amount of CO_2 sequestered from each facility. They are delivered to the sequestration sites (Eq. 24), which have maximum capacities (Eq. 25).

$$\sum_{(f,f',f'',t,l,q)\in FL} y_{f,f',f'',l,t,q} SQ_{f,f',f'',t,q} = SF_l \quad \forall l \in L^F \tag{23}$$

$$SF_l = \sum_{c\in C_{SQ}} \mathrm{seq}_{c,l} \quad \forall l \in L^F \tag{24}$$

$$\sum_{l\in L^F} \mathrm{seq}_{c,l} \leq \mathrm{SQCAP}_c \quad \forall c \in C_{SQ} \tag{25}$$

The objective function includes the total overall cost of the energy supply chain network, which covers (i) the investment costs associated with the new CBGTL plants, (ii) the electricity costs/gains, (iii) feedstock purchase and transportation costs, including the cost associated with expansion of transportation infrastructure, (iv) product transportation costs, (v) freshwater purchase and transportation costs, and (vi) sequestered CO_2 transportation and injection costs. Note that the electricity sales and purchases are treated separately in the objective function to allow a degree of flexibility for the system to sell or purchase electricity at different costs. These sales and purchases of electricity will occur at different locations throughout the country, meaning that even though on a nationwide basis there will be a net selling or purchasing of electricity, it does not necessarily mean that all selected facilities will uniformly sell or purchase electricity. For each supply chain network, there will be a combination of facilities that require or produce electricity in various locations. Thus, the objective function treats these two components separately, and the final value will reflect the net expenditure or gain from electricity net consumption/production for the supply chain.

$$\begin{aligned}&\sum_{l\in L^F}(\mathrm{Cost}_l^I - El_l^P\mathrm{Cost}^{El,P})\\&+\sum_{l\in L^F}(El_l^G\mathrm{Cost}^{El,G}+El_l^S\mathrm{Cost}^{El,S}+El_l^W\mathrm{Cost}^{El,W})\\&+\sum_{c\in C}\sum_{l\in L^F}w_{c,l}(\mathrm{Cost}_c^{WP}+\mathrm{Cost}_{c,l}^{WT})\\&+\sum_{c\in C}\sum_{l\in L^F}seq_{c,l}(\mathrm{Cost}_{c,l}^{CO_2,T}+\mathrm{Cost}_c^{CO_2,Inj})\\&+\sum_{(f,c,l,m)\in FT}x_{f,c,l,m}(\mathrm{Cost}_{f,c}^F+\mathrm{Cost}_{f,c,l,m}^{FT})\\&+\sum_{(p,c,l,m)\in PT}z_{p,l,c,m}\mathrm{Cost}_{p,l,c,m}^{PT}\end{aligned}\tag{26}$$

Equations 1–26 represent a large-scale mixed-integer linear optimization (MILP) model that can be solved using CPLEX. The model consists of 104,928 binary variables, 3,310,826 continuous variables, and 62,282 constraints, and is solved to obtain the active binary variables that represent the existence and selection of CBGTL facilities, the flow rates of feedstock and product, water, CO_2, electricity amounts in the supply chain topology. The computation is done on a single computer containing 8 Intel Xeon 2.83 GHz processors and shared memory parallelization, and the optimization model is solved using CPLEX and eight parallel threads. The large number of biomass resource locations that are close to each other causes the optimization problem to be degenerate. Thus, a decomposition strategy is employed in finding the best solution for the problem by first solving the optimization model with respect to coal and natural gas supply chains. Using a solution pool approach, multiple configurations of facility locations obtained from this step are used as initial points for the complete supply chain problem with the three carbon feedstocks. The best incumbent solutions are reported and the optimality gap for all performed computational studies ranges from 4-6%.

We investigated two categories of case studies of the optimal supply chain network, namely the network layouts that (a) replace 100%, 75%, and 50% of petroleum-based fuels and (b) utilize the locations of current energy infrastructures (i.e., coal mines and oil refineries). In the first category, the selections of the facility locations are not restricted to any physical constraints, and the economic performance is evaluated for the three levels of fuel replacements. In the second category, the facility locations are restricted to be at the locations of coal mines and oil refineries, and the model modifications can be found in Appendix B.

Results and Discussion

Replacement of petroleum-based fuels at 100%

The energy supply chain optimization model is first solved to achieve 100% replacement of petroleum-based fuels, resulting in 130 selected facilities in the supply chain network. The breakdown of the selected facilities consists of 9 small, 74 medium, and 47 large facilities, producing 0.68%, 28.05%, and 71.27% of the total fuels, respectively. Fuel production takes place mostly in large facilities due to economies of scale and the conversion levels of these facilities can be found in Table 1. Figure 1 is the graphical representation of the network layout, showing the locations of selected facilities overlaying the coal, biomass, and natural gas resources for the country. Notable clusters of large facilities are located in the central and southeast regions of the United States, where the three carbon feedstocks are in close proximity to the facility locations. The highest level of fuel production takes place in Kansas, which has 11

Table 1. Summary of Supply Chain Network Profile

Candidate Locations	Original Set	Original Set	Original Set	Coal Mines or Oil Refineries
Fuel replacement	100%	75%	50%	50%
Average fuel cost ($/bbl)	$95.11	$83.94	$75.83	$89.62
Total number of plants	130	109	66	94
Small	9	5	–	20
40	2	5	–	19
50	3	–	–	1
60	4	–	–	–
Medium	74	73	44	56
40	–	72	44	47
50	60	1	–	9
60	14	–	–	–
Large	47	31	22	18
40	–	27	22	15
50	25	4	–	3
60	22	–	–	–
Electricity				
Solar (MW)	–	–	–	–
Wind (MW)	–	–	–	–
Grid (MW)	99,977	1,274	–	1,575
Produced (MW)	165	74,627	54,040	45,316
Net required (MW)	99,812	−73,353	−54,040	−43,741
Water consumption (million gal/d)	664.4	585.3	387.7	369.2
CO_2 sequestered (million tonne/d)	2.96	2.68	1.79	1.80
Average GHG emissions (kg CO_2 eq./GJ)	32.45	9.18	5.16	5.36
Feedstock usage				
Coal (million short tons/yr)	1,012.5	1,007.61	730.55	701.70
Biomass (million tonnes/yr)	820.71	803.59	523.07	527.57
Natural gas (billion cf/yr)	5,791	5,761	3,923	3,847
Average investment costs per plant ($ billion)				
Small	$1.35	$1.33	–	$1.32
Medium	$4.46	$4.60	$4.57	$4.65
Large	$16.14	$16.08	$16.16	$16.29

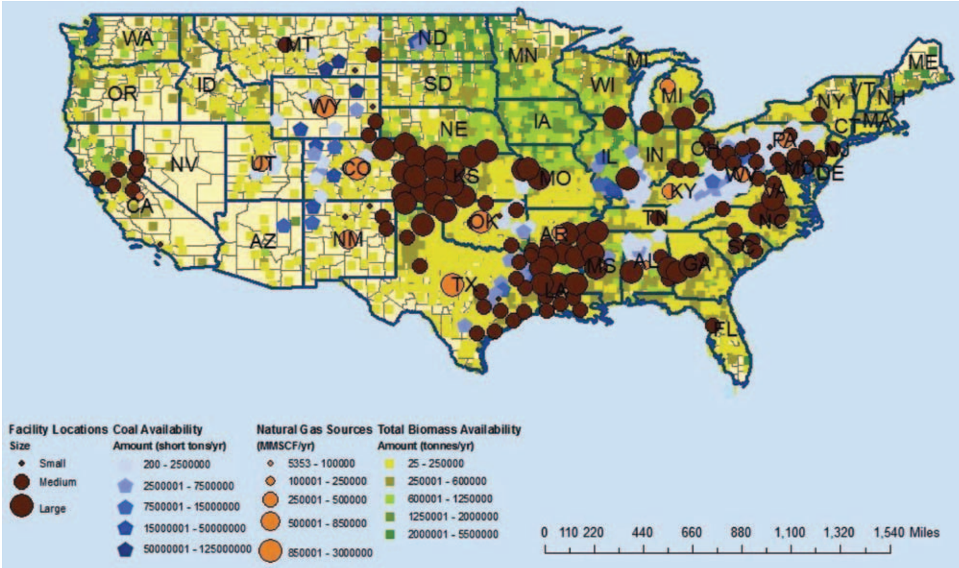

Figure 1. Graphical representation of the locations of selected facilities for 100% replacement of petroleum fuels.

The facilities are represented by dark brown circles centered at the proposed facility location with corresponding sizes. The amounts of coal, biomass, and natural gas feedstock in the United States are also represented using the proposed color scheme in the map legend. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

large facilities selected in its region. Texas has the highest number of selected facilities (1 small, 13 medium, 1 large), although due to the distributed nature of the biomass resources in Texas, most of the state's facilities are of medium capacity (see Supporting Information Table S7).

The overall cost of fuel production per barrel of crude oil equivalent is calculated to be \$95.11/bbl, with the plant investment costs being the highest contributing cost factor (41%), followed by biomass purchase (14%), and electricity cost (12%). The cost breakdown for this network is shown in Figure 2. The average cost, however, varies from state to state, and it is important to examine this profile since initial developments of the CBGTL network will naturally gravitate towards areas where fuels can be produced at a lower cost. The lowest costs are achieved in North Carolina (\$71.90/bbl), New Jersey (\$74.47/bbl), Florida (\$76.12/bbl), Tennessee (\$80.05/bbl), and Virginia (\$81.13/bbl), generally in the eastern part of the country. Kansas, where the highest level of fuel production takes place, averages at \$83.58/bbl. The highest costs are in Georgia (\$104.78/bbl), Texas (\$103.02/bbl), Arkansas (\$101.42/bbl), and Pennsylvania (\$98.80/bbl) (see Supporting Information Table S7).

Total biomass usage for the supply chain network amounts to 820.71 million dry tonnes/yr. This number falls between the estimated current availability of sustainable biomass of 460 million dry tonnes annual production and the projected production of 1 billion dry tones in the future.[30] The biomass feedstock is composed of 44.63% forest residues, 27.46% agricultural residues, and 27.91% perennial grasses. Almost all of the available forest residues are utilized (99.90%), with 45.90% of agricultural residues and 60.42% of perennial grasses utilized. The expansion for biomass production is due to the perennial grass requirement, which requires the future use of the conservation reserve program (CRP) land.[15] The coal usage, which amounts to 1,012.5 million short tons per year, compares to the United States production and consumption data, reported to be 1,072.8 and 1,000.4 million short tons in 2009, respectively.[34] Natural gas usage for the network (~5,791 billion cubic feet), on the other hand, is below current dry gas production, which is taken to be 20,580 billion cubic feet in 2009.[34]

A regional profile in the distribution of feedstock and products in the network emerges from the model solution, where local movements are preferred (see Supporting Information). Most of the facilities in the northeast and central regions satisfy most of their own coal requirement, while facilities in the southeast, midwest, and southwest receive coal from multiple regions. The western region receives coal from the central region in addition to using coal resources within the region.

The regional profile, however, is more pronounced in the biomass distribution, as most of it takes place within individual regions. The reason for this phenomenon is first attributed to the more distributed nature of biomass resources that allow for short-distance delivery. Since coal and natural gas are produced in a large-scale, centralized manner, inter-region delivery is often required. Second, biomass transportation cost is relatively higher compared to coal and natural gas on a per energy basis, favoring further the short-distance and intraregional transportation.

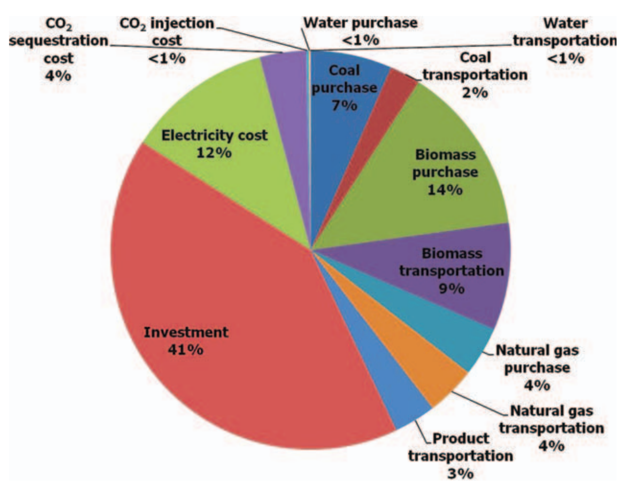

Figure 2. Cost breakdown for the entire supply chain network.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

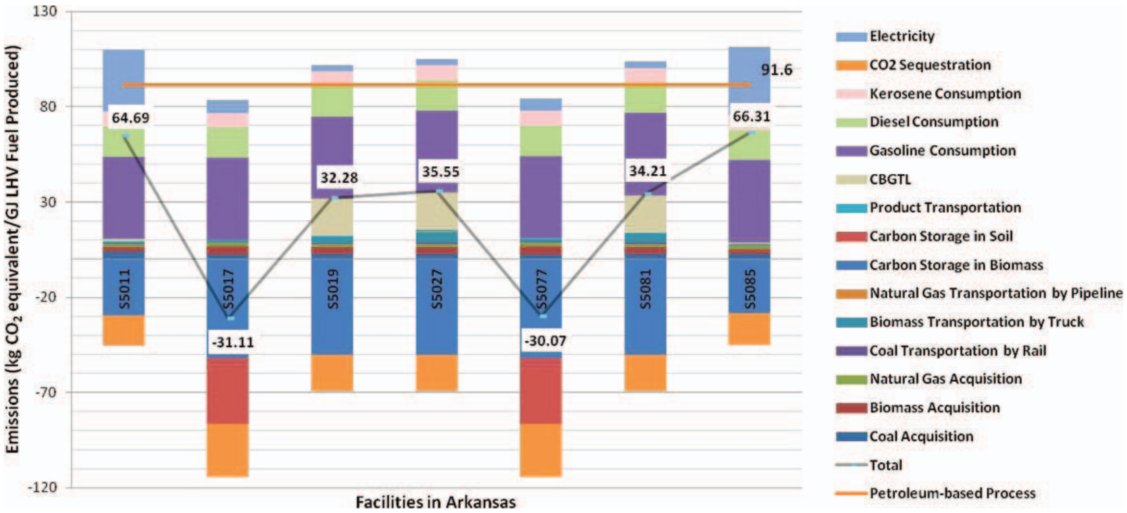

Figure 3. Breakdown of life cycle analysis for the greenhouse gas (GHG) emissions on seven selected facilities in the state of Arkansas.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Water consumption for the network is 664.4 million gallons per day, about 0.25% of freshwater withdrawal in the United States,[39] and 2.96 million tonne CO_2 is sequestered per day, which is at least three orders of magnitude less than the low estimate of total storage resource available given in Appendix C of the Atlas study.[40] Using a combination of carbon conversion levels, the network requires 99.98 GW from the grid, which is less than 10% of current grid capacity. Additionally, the network also produces 164.7 MW of electricity, due to the two small 40% conversion plants that exist in the network. Solar and wind electricity are not selected in the final solution due to their high investment costs in comparison to grid electricity or the electricity produced by the CBGTL facilities. The optimization solution indicates that it is more profitable to utilize grid electricity and to modify the selection of CBGTL facilities that require less or produce electricity to fulfill the maximum expansion limit, rather than utilizing solar or wind resources. If the maximum expansion of grid electricity is decreased, more solar or wind electricity would be utilized and a corresponding increase in the overall cost of fuel production is expected.

Figure 3 shows the breakdown of the LCA of seven representative plants in Arkansas into each of its contributing elements. It can be seen that the highest contributing factor of GHG emissions is the consumption of the liquid fuels, followed by, on some cases, the electricity usage. All fuel carbon is assumed to end up in the atmosphere upon consumption. These high emissions, however, are offset by the negative contributions from the carbon storage in biomass, CO_2 sequestration, and on facilities that utilize perennial grasses as feedstocks, the carbon storage in soil. The average emission for the entire network is 32.45 kg CO_2/GJ LHV, 35.4% of petroleum-bases fuels emission, which is made possible by the high usage of biomass in the supply chain.

Replacement of petroleum-based fuels at 75% and 50%

To observe the supply chain network layout when less amount of petroleum fuels are replaced, the mathematical model is solved for 75% and 50% fuel replacements. The geographical layouts of these case studies are shown in Figure 4. The overall fuel cost for the network decreases as the demand requirement is relaxed, amounting to \$83.94/bbl and \$75.83/bbl for 75% and 50% fuel replacements, respectively (see Table 1). The decrease in the number of plants with 50% and 60% carbon conversions corresponds with the decrease in the amount of electricity required from the grid, and the increased number of plants with 40% yields a higher amount of electricity produced from the supply chain network. The plants with 40% carbon conversions, however, require higher amounts of feedstocks. This trade-off is seen in the 75% fuel replacement case, where the supply chain network utilizes similar amounts of feedstocks as the 100% fuel replacement case but mostly using plants with 40% carbon conversions. This shift results in a net production of 73.3 GW of electricity, compared to 99.8 GW of electricity consumption in the 100% fuel replacement case.

The plants with 40% carbon conversions also have higher coal contribution in the feedstock compositions. As coal is the cheapest among the three carbon feedstocks, the supply chain selects a higher coal contribution to drive down the overall cost of fuel production. Thus, the 75% fuel replacement case utilizes a high amount of coal feedstock. When more liquid fuels need to be produced with the same amount of coal availabilities in the 100% fuel replacement case, plants with 50% and 60% carbon conversions are selected in the supply chain network that can produce liquid fuels with less amounts of carbon feedstocks.

When 50% of petroleum fuel is replaced, the supply chain network is comprised of 66 plants (44 medium and 22 large), all of which are plants with 40% carbon conversion. All of these plants produce electricity, amounting to 54.04 GW produced for the entire country. For 50% replacement of petroleum-based fuels, reduction in feedstocks utilization is achieved, with annual consumptions of 730.55 million short tons for coal, 523.07 million dry tonnes for biomass, and 3,923 billion cubic feet for natural gas.

The GHG average emissions for the 75% and 50% fuel replacements case studies are 9.18 and 5.16 kg CO_2 eq./GJ, respectively (see Table 1). Note that these average emissions are calculated based on the amount of fuels produced by the CBGTL supply chain. In other words, the remaining 25% and 50% liquid fuels are still based on petroleum processes and have petroleum-based emissions, and the overall average emissions for the entire United States would be higher than the values listed in Table 1.

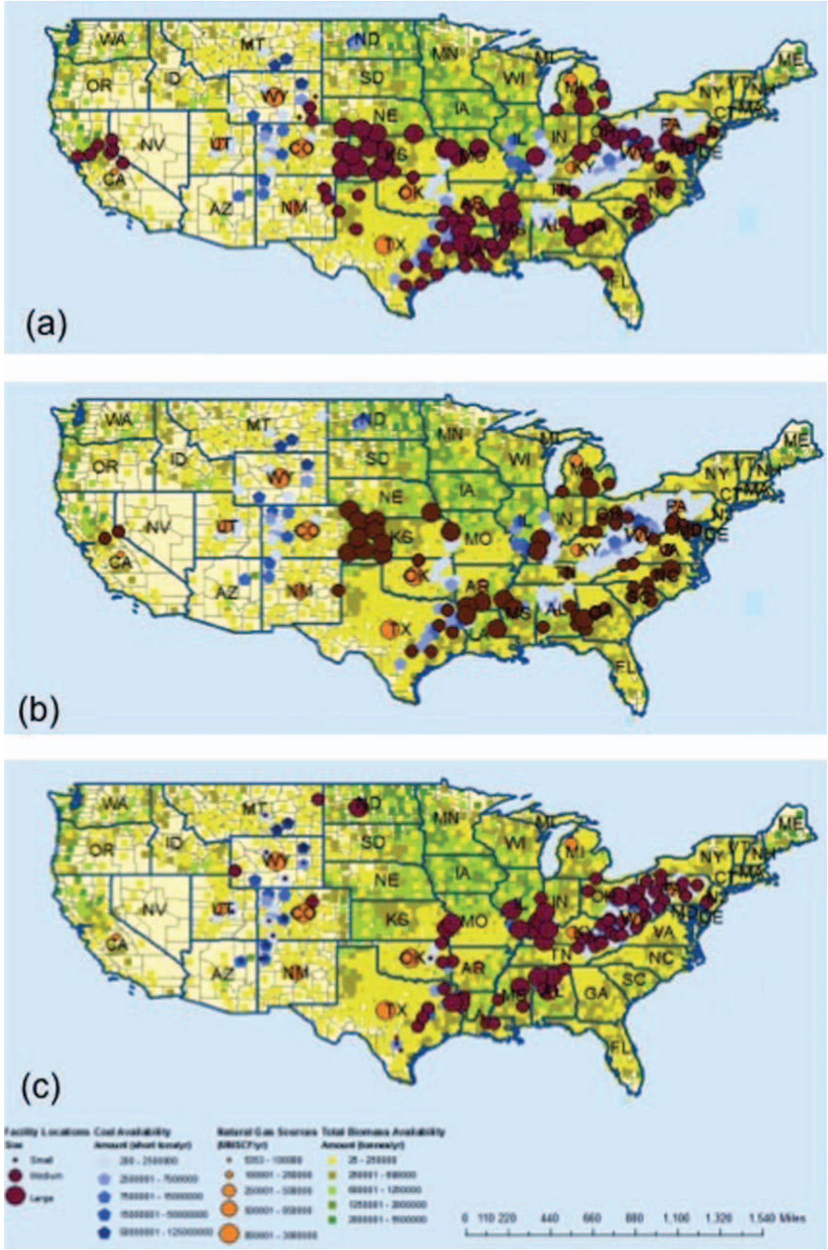

Figure 4. Graphical representation of the locations of selected facilities for (a) 75% replacement of petroleum fuels, (b) 50% replacement of petroleum fuels, and (c) 50% replacement of petroleum fuels with a reduced set of candidate locations (i.e., either at coal mines or oil refineries).

The facilities are represented by dark brown circles centered at the proposed facility location with corresponding sizes. The amounts of coal, biomass, and natural gas feedstock in the United States are also represented using the proposed color scheme in the map legend. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Towards utilization of existing infrastructures

To explore the supply chain network that utilizes existing infrastructure, namely locations of oil refineries and coal mines, a case study is completed where the locations of CBGTL facilities have to coincide with the locations of coal mines or oil refineries by incorporating the modifications to the mathematical model given in Appendix B. Table 1 records the summary of the supply chain profile, showing that 50% fuel replacements can be achieved with the reduced set of candidate locations. A total of 94 plants are selected with a net electricity production of 43.74 GW for the entire country, due to the highly selected 40% carbon conversion plants.

Compared with the original set of candidate locations, placing facilities at existing coal mines and oil refineries incurs higher overall cost ($89.62/bbl, compared to $75.83/bbl) due to the increased distances in natural gas and fuel products transportation. The selection of facility locations favor the coal mines site (see Figure 4), preferring the infrastructure for the feedstock supply to the infrastructure for liquid fuel product distribution, and the selected 40% carbon conversion plants have higher coal contribution in their feedstock compositions. Overall, reduced utilizations of feedstock resources are observed, namely 701.70 million short tons for coal, 527.57 million dry tonnes for biomass, and 3,847 billion cubic feet for natural gas.

To implement the results presented in this article, several other factors need to be considered, such as the temporal aspect of building CBGTL facilities for sequential replacement of petroleum fuels over a long time horizon. In this article, we ask the existence question to investigate the feasibility, economic, and environmental performance of an energy supply chain network for liquid transportation fuels based on domestically available coal, biomass, natural gas, and the CBGTL process. The temporal aspect of the supply chain problem, including questions on which facilities should be built first, at what locations, capacities, and their profitabilities, need to be addressed in a strategic planning framework, which is the subject of our on-going and future work.

Conclusions

The supply chain optimization framework proposed in this article highlights an approach that can integrate the features of multiple sectors into consideration and optimize a network of hybrid energy facilities with respect to all of their upstream and downstream operations. The mathematical model is flexible in that the users can determine the granularity of each set of parameter inputs (e.g., more discretized natural gas locations, developing CO_2 sequestration sites, etc) as they become available and obtain better quality solutions. The analyzed results in this study suggest that the hybrid CBGTL supply chain has potential to satisfy the United States transportation fuel demands with domestically available resources with significant environmental gains compared to petroleum-based fuels.

Acknowledgments

The authors acknowledge partial financial support from the National Science Foundation (NSF EFRI-0937706).

Notation

Index

- s = state index
- c = county index
- f = feedstock index
- p = product index
- t = plant size index
- l = plant location index
- m = transportation mode index
- r = port index
- q = carbon conversion level index

Sets

- S = U.S. states
- C = U.S. counties
- F^B = biomass feedstocks (i.e., forest residues, agricultural residues, perennial grasses)
- F^C = coal feedstocks (i.e., HV bituminous, MV bituminous, LV bituminous, subbituminous, lignite, anthracite)
- F^G = natural gas feedstocks
- F = feedstocks
- FC = feedstock triplets
- P = products (i.e., gasoline, diesel, kerosene)
- C_F = feedstock-county pairs
- C_P = product-county pairs
- C_{SQ} = carbon sequestration sites
- C_W = locations of water resources
- L^F = candidate plant locations
- L^S = candidate locations with solar plant capacities
- L^W = candidate locations with wind plant capacities
- M = modes of transportation (i.e., truck, rail, pipeline, barge)
- M_F = feedstock-mode pairs
- M_P = product mode pairs
- M^G_{Pipe} = natural gas pipelines
- M^P_{Pipe} = product pipelines
- R = 50 U.S. ports with high liquid fuels capacity
- T = plant sizes (i.e., small, medium, large)
- Q = carbon conversion levels (i.e., 40%, 50%, 60%)
- EFL = enumerated facility locations
- FL = filtered facility locations
- FT = feasible feedstock flow quadruplets
- PT = feasible product flow quadruplets

Set Definitions

- $f \in F = F^B \cup F^C \cup F^G$
- $FC = \{(f,f',f'') | f \in F^C, f' \in F^B, f'' \in F^G\}$
- $M_F = \{(f,m) \in F^B \times \text{truck} \cup F^C \times \{\text{rail}\} \cup F^G \times \text{pipeline}\}$
- $M_P = \{(p,m) \in P \times \{\text{pipeline,truck,barge}\}\}$
- $EFL = \{(f,f',f'',t,l,q) \in FC \times T \times L \times Q\}$
- $FT = \{(f,c,l,m) | (f,c) \in C_F,\ l \in L,\ (f,m) \in M_F,\ \text{Cost}^{FE}_{f,c,l,m} \le \text{MaxCost}^{FE}_f\}$
- $PT = \{(p,l,c,m) | (p,c) \in C_P,\ l \in L,\ (p,m) \in M_P,\ \text{Cost}^{PE}_{p,c,l,m} \le \text{MaxCost}^{PE}_p\}$
- $C_F = \{(f,c) | (f,c) \in F \times C, FA_{f,c} > 0\}$
- $C_P = \{(p,c) | (p,c) \in P \times C, DM_{p,c} > 0\}$
- $C_W = \{c | c \in C, WA_c > 0\}$
- $C_{SQ} = \{c | c \in C, \text{SCAP}_c > 0\}$
- $L^S = \{l | l \in L^F, \text{Cap}^S_l > 0\}$
- $L^W = \{1 | l \in L^F, \text{Cap}^W_l > 0\}$

Parameters

- Prod_t = amount of total fuel products for CBGTL plant size t
- Ratio_p = relative proportion of product p from CBGTL plant
- N = Maximum number of CBGTL plants built in the United States
- $N^{\max}_t$ = maximum number of CBGTL plants for size t
- $N^{\min}_t$ = minimum number of CBGTL plants for size t
- $LC_{f,f',f'',t,q}$ = CBGTL levelized investment cost for feed combination (f,f',f''), size t, and carbon conversion option q
- $FR^C_{f,f',f'',t,q}$ = CBGTL coal requirement for feed combination (f,f',f''), size t, and carbon conversion option q
- $FR^B_{f,f',f'',t,q}$ = CBGTL biomass requirement for feed combination (f,f',f''), size t, and carbon conversion option q
- $FR^G_{f,f',f'',t,q}$ = CBGTL natural gas requirement for feed combination (f,f',f''), size t, and carbon conversion option q
- $ER_{f,f',f'',t,q}$ = CBGTL electricity requirement for feed combination (f,f',f''), size t, and carbon conversion option q
- $EP_{f,f',f'',t,q}$ = CBGTL electricity produced for feed combination (f,f',f''), size t, and carbon conversion option q
- $FW_{f,f',f'',t,q}$ = CBGTL freshwater requirement for feed combination (f,f',f''), size t, and carbon conversion option q
- $SQ_{f,f',f'',t,q}$ = CBGTL CO_2 sequestration flow for feed combination (f,f',f''), size t, and carbon conversion option q
- $FA_{f,c}$ = availability of feedstock f in county c
- $DM_{p,c}$ = demand of product p in county c
- WA_c = water availability in location c
- SCAP_c = CO_2 sequestration capacity in location c
- MaxCost^{FE}_f = maximum delivered cost of feedstock f
- MaxCost^{PE}_p = maximum delivered cost of product p
- Cap^S_l = maximum capacity of solar generated electricity at location l
- Cap^W_l = maximum capacity of wind generated electricity at location l
- Cap^G = maximum grid electricity usage for the country
- Cap_m = flow capacity of natural gas interstate pipeline m
- Usage_m = average daily flow currently in use for the natural gas interstate pipeline m
- $\text{Cost}^F_{f,c}$ = cost per unit mass of feedstock f at county c
- $\text{Cost}^{FT}_{f,c,l,m}$ = cost per unit mass flow to transport feedstock f from county c to facility l using mode m
- $\text{Cost}^{PT}_{p,l,c,m}$ = cost per unit mass flow to transport product p from facility l to county c using mode m
- $\text{Cost}_{El,G}$ = total investment cost per unit energy of grid electricity
- $\text{Cost}_{El,P}$ = total profit per unit energy of produced electricity
- $\text{Cost}_{El,S}$ = total investment cost per unit energy of solar electricity
- $\text{Cost}_{El,W}$ = total investment cost per unit energy of wind electricity
- Cost^{WP}_c = cost of water purchase at location c per unit flow rate

$\text{Cost}_{c,l}^{WT}$ = cost of water transportation by pipeline from source c to facility l
$\text{Cost}_{c,l}^{CO_2,T}$ = Cost of CO_2 transportation by pipeline from facility l to sequestration cite c
$\text{Cost}_{c}^{CO_2,Inj}$ = Cost of CO_2 injection at sequestration cite c

Note that the parameter values for FA for biomass feedstock are modified from Elia et al. (2011)[15] accordingly, as described in the main text. The species members of each biomass category in Elia et al. (2011)[15] are lumped together and modeled as three representative biomass types with their corresponding availabilities and purchase costs.

Continuous Variables

Cost_l^I = levelized investment cost of facility l
$FR_{f,l}$ = amount of feedstock f required at facility l
El_l^T = total electricity required at facility l
El_l^P = total electricity produced at facility l
El_l^S = solar electricity required at facility l
El_l^W = wind electricity required at facility l
El_l^G = grid electricity required at facility l
WF_l = freshwater requirement for facility l
SF_l = sequestered CO_2 amount from facility l
$w_{c,l}$ = freshwater flow from source c to facility l
$\text{seq}_{c,l}$ = CO_2 sequestration flow from facility l to injection site c
$x_{f,c,l,m}$ = flow of feedstock f from county c to facility l using transportation mode m
$z_{p,l,c,m}$ = flow of product p from facility l to county c using transportation mode m

Binary Variables

$y_{f,f',f'',t,l,q}$ = CBGTL plant binary at location l with feed combination (f,f',f''), size t, and carbon conversion option q

Literature Cited

1. Floudas CA, Elia JA, Baliban RC. Hybrid and single feedstock energy processes for liquid transportation fuels: a critical review. *Comp Chem Eng* 2012;41:24–51.
2. Agrawal R, Singh NR, Ribeiro FH, Delgass WN. Sustainable fuel for the transportation sector. *Proc Natl Acad Sci USA*. 2007;104:4828–4833.
3. Takeshita T, Yamaji K. Important roles of Fischer-Tropsch synfuels in the global energy future. *Energy Policy*. 2008;36:2773–2784.
4. Kreutz TG, Larson ED, Liu G, Williams RH. *Fischer-Tropsch fuels from coal and biomass*. In. *Proceedings of the 25th Annual International Pittsburgh Coal Conference*. Pittsburgh, PA, 2008. Available at web.mit.edu/mitei/docs/reports/kreutz-fischer-tropsch.pdf.
5. Liu G, Larson ED, Williams RH, Kreutz TG, Guo X. Making Fischer-Tropsch fuels and electricity from coal and biomass: performance and cost analysis. *Energy Fuels*. 2011;25:415–437.
6. Larson ED, Fiorese G, Liu G, Williams RH, Kreutz TG, Consonni S. Coproduction of decarbonized synfuels and electricity from coal + biomass with CO_2 capture and storage: an Illinois case study. *Energy Environ Sci*. 2010;3:28–42.
7. Tilman D, Hill J, Lehman C. Carbon-negative biofuels from low-input high-diversity grassland biomass. *Science*. 2006;314:1598–1600.
8. Sudiro M, Bertucco A. Production of synthetic gasoline and diesel fuel by alternative processes using natural gas and coal: process simulation and optimization. *Energy*. 2009;34:2206–2214.
9. Adams TA, II, Barton PI. Combining coal gasification and natural gas reforming for efficient polygeneration. *Fuel Proc Tech*. 2011;92:639–655.
10. Weekman VW. Gazing into an energy crystal ball. *Chem Eng Prog*. 2010;106:23–27.
11. Martin M, Grossmann IE. Process optimization of FT-diesel production from lignocellulosic switchgrass. *Ind Eng Chem Res*. 2011;50:13485–13499.
12. National Academy of Sciences, National Academy of Engineering, and National Research Council. Liquid Transportation Fuels from Coal and Biomass: Technological Status, Costs, and Environmental Issues. 2009. Available at www.nap.edu/catalog.php?record_id=12620.
13. Baliban RC, Elia JA, Floudas CA. Toward novel biomass, coal, and natural gas processes for satisfying current transportation fuel demands, 1: process alternatives, gasification modeling, process simulation, and economic analysis. *Ind Eng Chem Res*. 2010;49:7343–7370.
14. Elia JA, Baliban RC, Floudas CA. Toward novel biomass, coal, and natural gas processes for satisfying current transportation fuel demands, 2: simultaneous heat and power integration. *Ind Eng Chem Res*. 2010;49:7371–7388.
15. Elia JA, Baliban RC, Xiao X, Floudas CA. Optimal energy supply network determination and life cycle analysis for hybrid coal, biomass, and natural gas to liquid (CBGTL) plants using carbon-based hydrogen production. *Comp Chem Eng*. 2011;35:1399–1430.
16. Baliban RC, Elia JA, Floudas CA. Optimization framework for the simultaneous process synthesis, heat and power integration of a thermochemical hybrid biomass, coal, and natural gas facility. *Comp Chem Eng*. 2011;35:1647–1690.
17. Baliban RC, Elia JA, Floudas CA. Simultaneous process synthesis, heat, power, and water integration of thermochemical hybrid biomass, coal, and natural gas facilities. *Comp Chem Eng*. 2012;37:297–327.
18. Baliban RC, Elia JA, Misener R, Floudas CA. Global optimization of a MINLP process synthesis model for thermochemical based conversion of hybrid coal, biomass, and natural gas to liquid fuels. *Comp Chem Eng*. doi:10.1016/j.compchemeng.2012.03.008.
19. Gold S. Bio-energy supply chains and stakeholders. *Mitigation Adapt Strategies Global Change*. 2011;16:439–462.
20. Lam HL, Varbanov PS, Klemeš JJ. Regional renewable energy and resource planning. *Appl Energy*. 2011;88:545–550.
21. Richard TL. Challenges in scaling up biofuels infrastructure. *Science*. 2010;329:793–796.
22. Somerville C, Youngs H, Taylor C, Davis SC, Long SP. Feedstocks for lignocellulosic biofuels. *Science*. 2010;329:790–792.
23. Ravula PP, Grisso RD, Cundiff JS. Cotton logistics as a model for a biomass transportation system. *Biomass Bioenergy*. 2008;32:314–325.
24. Kumar A, Cameron JB, Flynn PC. Biomass power cost and optimum plant size in western Canada. *Biomass Bioenergy*. 2003;24:445–464.
25. Dal-Mas M, Giarola S, Zamboni A, Bezzo F. Strategic design and investment capacity planning of the ethanol supply chain under price uncertainty. *Biomass Bioenergy*. 2011;35:2059–2071.
26. Huang Y, Chen CW, Fan Y. Multistage optimization of the supply chains of biofuels. *Transport Res Part E*. 2010;46:820–830.
27. Cundiff JS, Fike JH, Parrish DJ, Alwang J. Logistic constraints in developing dedicated large-scale bioenergy systems in the Southeastern United States. *J Environ Eng-ASCE*. 2009;135:1086–1096.
28. Parker N, Tittmann P, Hart Q, Nelson R, Skog K, Schmidt A, Gray E, Jenkins B. Development of a biorefinery optimized biofuel supply curve for the Western United States. *Biomass Bioenergy*. 2010;34:1597–1607.
29. Liu P, Whitaker A, Pistikopoulos EN, Li Z. A mixed-integer programming approach to strategic planning of chemical centers: a case study in the UK. *Comp Chem Eng*. 2011;35:1359–1373.
30. Department of Energy and U.S. Department of Agriculture. Biomass as Feedstock for a Bioenergy and Bioproducts Industry: The Technical Feasibility of a Billion-Ton Annual Supply. 2005. Available at www1.eere.energy.gov/biomass/pdfs/final_billionton_vision_report2.pdf.
31. National Energy Technology Laboratory. Quality Guidelines for Energy System Studies. 2004. Available at www.netl.doe.gov/technologies/coalpower/gasification/pubs/market.html.
32. Baños R, Manzano-Agugliaro F, Montoya FG, Gil C, Alcayde A, Gómez J. Optimization methods applied to renewable and sustainable energy: a review. *Renewable Sustainable Energy Rev* 2011;15:1753–1766.
33. Ministry of Foreign Affairs of Japan. G8 Hokkaido Toyako Summit Leaders Declaration. 2008.
34. Energy Information Administration. Annual Energy Outlook 2010. Available at http://www.eia.doe.gov/oiaf/aeo/. 2010.
35. National Renewable Energy Laboratory. National Solar Radiation Database 1991-2005 Update: User's Manual. Contract No. DE-AC36-99-GO10337. 2007.
36. National Renewable Energy Laboratory. Wind Integration Datasets. 2010. Available at www.nrel.gov/wind/integrationdatasets.
37. Department of Energy. Energy Demands on Water Resources. 2006. Available at www.sandia.gov/energy-water/docs/121-RptToCongress-EWwEIAcomments-FINAL.pdf.
38. Mielke E, Anadon LD, Narayanamurti V. *Water Consumption of Energy Resource Extraction, Processing, and Conversion*. 2010. Available at belfercenter.ksg.harvard.edu/files/ETIP-DP-2010-15-final-4.pdf.
39. Kenny JF, Barber NL, Hutson SS, Linsey KS, Lovelace JK, Maupin MA. *Estimated Use of Water in the United States in 2005*, U.S. Geological Survey. 2009.

40. National Energy Technology Laboratory. *NETL 2010 Carbon Sequestration Atlas of the United States and Canada*, 3rd ed. Atlas III. 2010. Available at www.netl.doe.gov/technologies/carbon_seq/refshelf/atlas/.
41. Ogden JM. Conceptual design of optimized fossil energy systems with capture and sequestration of carbon dioxide. 2004. Available at pubs.its.ucdavis.edu/publication_detail.php?id=196.
42. Argonne National Laboratory. *GREET 1.8b, The Greenhouse Gases, Regulated Emisssions, and Energy Use in Transportation (GREET) Model*. 2007. Available at greet.es.anl.gov.

Appendix A: Candidate Facility Locations

The following methodologies are used to determine a set of candidate facility locations throughout the United States. The complete list of index, set, and parameter definitions can be found in the Notation section. Initially, every county centroid is postulated to be a potential plant location. This list is subsequently reduced by applying elimination criteria to filter out locations that are deemed unsuitable. The United States is comprised of 3,136 counties and the set of all possible locations of the CBGTL plants is defined as follows.

$$l \in L = \{\text{United States counties}\}$$

We define the set of connections (FT) that consist of the counties c that can deliver feedstock f via transportation mode m to facility location l as follows.

$$FT = \{(f,c,l,m) \mid (f,c) \in C_F, l \in L, (f,m) \in M_F\}$$

The feedstock connections and the candidate facilities are first filtered using maximum transportation cost ($\text{Cost}^{\text{Trans}}$) criteria, imposed such that coal and natural gas transportation can travel greater distances than biomass transportation. Biomass is transported by truck, coal is transported by rail, and natural gas is transported via interstate and intrastate pipelines. The connection between a feedstock location and a facility location is not allowed when the associated transportation cost is more than the imposed limits. Note that these filters naturally exclude Hawaii and Alaska as candidate locations for the CBGTL facilities, since the feedstock transportation to and from these states are prohibitive.

Subsets of FT for biomass, coal, and natural gas feedstocks are defined as follows.

$$\begin{aligned} FT^B = \{&(f,c,l,m) \mid (f,c) \in C_F^B, l \in L, \\ &(f,m) \in F^B \times \text{truck}, \text{Cost}^{\text{Trans}}_{f,c,l,m} \le \$2.00/\text{GJ}\} \\ FT^C = \{&(f,c,l,m) \mid (f,c) \in C_F^C, l \in L, \\ &(f,m) \in F^C \times \text{rail}, \text{Cost}^{\text{Trans}}_{f,c,l,m} \le \$10.00/\text{GJ} \\ FT^G = (&f,c,l,m) \mid (f,c) \in C_F^G, l \in L, \\ &(f,m) \in F^G \times \text{pipeline}, \text{Cost}^{\text{Trans}}_{f,c,l,m} \le \$10.00/\text{GJ}\} \end{aligned}$$

Based on the established connections, we define subsets of facility locations L^B, L^C, and L^C defined as locations that can receive biomass, coal, and natural gas within the cost limitations, accounting to 3,136, 2,866, and 2,493 counties, respectively. A facility location, however, must be able to receive all three feedstocks within the imposed criteria. Thus, we define a set L^F in the following equation.

$$L^F = \{l \mid L^B \cap L^C \cap L^G\}$$

The number of locations in set L^F is equal to 1880 counties.

All 1880 counties then are ranked separately based on the amount of coal, biomass, and natural gas produced in each county. Thus, each county is associated with three ranking values associated with each feedstock, and a final rank order list is constructed based on the combined coal, biomass, and natural gas rankings. Based on this rank order list, we can select the top N number of counties for each state that can serve as a potential CBGTL facility site. A parametric analysis was completed to determine what N should be, taking the top 10–100% of the 1880 potential sites in 10% increment (e.g., if 10% is considered, we take the ceiling of the 10% of the total potential sites on a per state basis). Trade-offs between the improved value of the objective function, increased computational time, and model complexity with the increased number of candidate locations were examined and it was determined that the top 70% sites on a per state basis gave the best results. The reduced set L^F then is comprised of 1329 candidate locations for the CBGTL supply chain network.

Appendix B: Model Modification

When coal mines or oil refineries are used as candidate locations, the following modifications to the model apply. we define additional sets OL and CL as follows.

$$\begin{aligned} OL = \{&(l) \mid l \in L, l \text{ is an} \\ &\text{oil refinery location.}\} \end{aligned} \tag{B1}$$

$$\begin{aligned} CL = \{&(l) \mid l \in L, l \text{ is a} \\ &\text{coal mine location.}\} \end{aligned} \tag{B2}$$

Set OCL is defined as the union of OL and CL, representing a list of locations that are close to either oil refineries or coal mines.

$$OCL = OL \cup CL \tag{B3}$$

The total fuel demand for the United States, TDM is defined as follows.

$$TDM_p = \sum_{(c) \in C} DM_{p,c} \quad \forall (p) \in P \tag{B4}$$

To enforce that a portion of the demand must be fulfilled by facilities located in the proximity of coal mines or oil refineries, the following constraints are added to the original mathematical model.

$$\begin{aligned} FP \cdot TDM_p = &\sum_{(f,f',f'',t,l,q) \in FL} y_{f,f',f'',l,t,q} \text{Prod}_t \text{Ratio}_p \\ &\forall l \in OL, p \in P \end{aligned} \tag{B5}$$

$$\begin{aligned} FP \cdot TDM_p = &\sum_{(f,f',f'',t,l,q) \in FL} y_{f,f',f'',l,t,q} \text{Prod}_t \text{Ratio}_p \\ &\forall l \in CL, p \in P \end{aligned} \tag{B6}$$

$$\begin{aligned} FP \cdot TDM_p = &\sum_{(f,f',f'',t,l,q) \in FL} y_{f,f',f'',l,t,q} \text{Prod}_t \text{Ratio}_p \\ &\forall l \in OCL, p \in P \end{aligned} \tag{B7}$$

where FP is the fuel proportion that is enforced according to each case study.

Manuscript received Mar. 27, 2012, and revision received May 3, 2012.