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Shale Gas Supply Chain Design and Operations toward Better Economic and Life Cycle Environmental Performance: MINLP Model and Global Optimization Algorithm

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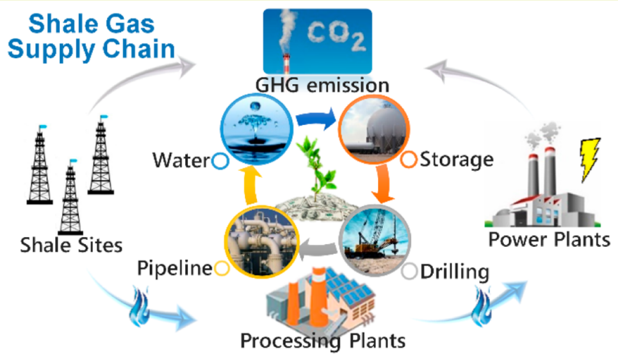
Supporting Information

ABSTRACT: In this work, the life cycle economic and environmental optimization of shale gas supply chain network design and operations is addressed. The proposed model covers the well-to-wire life cycle of electricity generated from shale gas, consisting of a number of stages including freshwater acquisition, shale well drilling, hydraulic fracturing and completion, shale gas production, wastewater management, shale gas processing, electricity generation as well as transportation and storage. A functional-unit based life cycle optimization problem for a cooperative shale gas supply chain is formulated as a multi-objective nonconvex mixed-integer nonlinear programming (MINLP) problem. The resulting Pareto-optimal frontier reveals the trade-off between the economic and environmental objectives. A case study based on Marcellus shale play shows that the greenhouse gas emission of electricity generated from shale gas ranges from 433 to 499 kg CO_2e/MWh, and the levelized cost of electricity ranges from \$69 to \$91/MWh. A global optimization algorithm is also presented to improve computational efficiency.



KEYWORDS: *Sustainable supply chain, Life cycle optimization, Shale gas, MINLP, Global optimization*

INTRODUCTION

Natural gas is an important carrier used to meet global energy demand. In recent years, accompanying the advances in horizontal drilling and hydraulic fracturing, shale gas, or natural gas extracted from shale rock, has emerged as a promising energy source. In the U.S., the shale gas production contribution to total natural gas production has increased from less than 5% to 35% from 2005 to 2012, and it is expected to reach 50% by 2035.[1,2] The shale gas production system is a complex multistage network and includes various components such as water acquisition, shale gas production, wastewater management, shale gas processing, inventory, usage, and transportation. A variety of decisions must be made in each stage of this system. Hence, discerning the optimal design and operations of the shale gas supply chain has great economic potential.[3] Meanwhile, the environmental performance of shale gas is of great concern. Natural gas is mainly composed of methane, which is about 25 times more potent as a greenhouse gas (GHG) than carbon dioxide based on the 100-year global warming potential (GWP). Thus, small rates of methane emissions could have a large influence on the greenhouse gas footprints of natural gas use.[4−7] Moreover, supply chain activities such as shale gas production, processing, transportation, and power generation could also incur large amount of GHG emissions. Therefore, climate benefits of shale gas compared to traditional fossil fuels depend on overall GHG emission of the whole system. Due to significant expected economic and environmental impacts, it is essential to simultaneously take both of these criteria into account when addressing the optimal design and operations of a shale gas supply chain.

There are publications addressing the design and operations of shale gas supply chains in the existing literature, while few of them provide a systematic way to address both the economic and environmental impacts associated with shale gas production.[8−12] Yang and Grossmann[13] present a mixed-integer linear programming (MILP) model to maximize the economics of water use in hydraulic fracturing. Cafaro and Grossmann[14] present a mixed-integer nonlinear programming (MINLP) model to optimally determine the most economical design of a shale gas supply chain. However, they did not take into account the actual lifetime of shale wells. Gao and You[15] propose a mixed-integer linear fraction programming (MILFP) model to address the optimal design and operations of water supply chain networks for shale gas production. Apart from literature focusing on the design and operations of shale gas

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supply chains, there are a growing number of publications that regard environmental impacts, especially the life cycle carbon footprint of shale gas, to evaluate the sustainability of this energy resource. In 2011, Howarth et al.[16] present an analysis of the GHG footprint of shale gas. This work spurred a large increase in research and analysis on the life cycle carbon footprint of shale gas using different data and assumptions.[1,4,17−26] Weber and Clavin[27] present a review of the original study from Howarth as well as the subsequent studies. Heath et al.[28] present a harmonization method to develop robust and updated comparisons of life cycle GHG emissions for electricity produced from shale gas, conventional natural gas, and coal. Allen[5] recommends reconciling bottom-up and top-down measurements for a better understanding of methane emissions from a natural gas supply chain.

A shortage of decision-support tools and methodologies dedicated to the sustainable design and operations of a shale gas supply chain systems can be identified from the review of existing work in the field. Thus, the main goal of this work is to develop a functional-unit based life cycle optimization model for optimal design and operations of a shale gas supply chain, which simultaneously evaluates and optimizes the economic and GHG emission by optimization of decisions for network design, drilling scheduling, technology selection, facility location and sizing, natural gas storage, and transportation, etc. To address this challenging problem, a multiobjective, multiperiod nonconvex MINLP model is proposed, which features fractional-form objective function involving nonlinear terms to account for the functional unit of this study. It is worth noting that the amount of GHG emissions is chosen as the only environmental indicator in this work due to available environmental impact data for shale gas. Almost all of the existing LCA studies on shale gas focus on GHG emissions.[4,20−24,27,29−33] The noncooperative supply chain optimization problem is very challenging to tackle with the state-of-the-art mathematical programming techniques, so a cooperative model is assumed in this work following the pattern of most existing life cycle optimization work.[34−38] In the proposed life cycle optimization model, the seasonality of freshwater supply, scheduling of shale well drilling, wastewater management, shale gas processing, underground storage, electric power generation, and transportation are all considered. Levelized cost of the electricity (LCOE) generated from shale gas is chosen as the economic indicator for the projected economic performance of the shale gas supply chain. The GHG emissions per unit amount of electricity from shale gas is chosen as the environmental indicator, which is evaluated based on the well-to-wire life cycle assessment (LCA).[27] Because of the combinatorial nature and nonconvexity of the MINLP problem, it is very challenging to globally optimize the large-scale supply chain problems. To address this issue, a global optimization method is presented that integrates the parametric algorithm with a branch-and-refine method that is much more efficient than general-purpose MINLP solvers.

The major novelties of this work are summarized: (1) A novel and comprehensive multiperiod MINLP model for the design and operations of shale gas supply chain network incorporating with water supply chain network is formulated. (2) Simultaneous life cycle optimization of economic and environmental impacts of shale gas supply chain based on a standardized functional unit is performed. (3) This model is applied to a specific case study based on the Marcellus shale play.

■ PROBLEM STATEMENT

In general, the problem addressed in this work can be stated as follows. A planning horizon is given that is approximately equal to the lifetime of the shale well and divided into a set of intermediate time periods. Multiple wells can be drilled at a single shale site with horizontal drilling techniques. Shale sites will acquire freshwater for drilling and hydraulic fracturing operations from a set of freshwater sources. In each shale well, millions of gallons of fracturing fluid are pumped into the wellbore under high pressure. Thus, fractures are created and held open in the shale rock layer, making it easier to extract shale gas and oil.[39] Along with the production of raw shale gas, a certain percentage of water injected underground flows back to the surface as highly contaminated wastewater. There is a significant amount of such wastewater that is challenging to treat.[40] Generally, there are three wastewater management options, including centralized wastewater treatment (CWT), onsite treatment for reuse, and deep injection disposal wells.[41−43] Wastewater from shale gas production can be transported to CWT facilities for treatment and then discharged to surface water. Onsite treatment for reuse involves different technologies of pretreatment, namely multistage flash (MSF), multieffect distillation (MED), and reverse osmosis (RO) units. The pretreated water can be blended with freshwater and can be reused for drilling or hydraulic fracturing again. In addition, wastewater can be transported to Class-II disposal wells and pumped underground without any treatment. Pennsylvania currently has seven disposal wells, and transporting wastewater to some out-of-state disposal wells, for example those in Ohio, can be less attractive due to long-distance transportation costs.[3] The shale gas production profile of the shale well at each shale site is assumed to be known and decreases along with time, as depicted in Figure S6 of the Supporting Information.[14] The raw gas extracted from the shale gas formations is transported from well sites to processing plants through pipelines, where contaminants such as water and other compounds are removed, and higher density hydrocarbons and natural gas are separated. The shale gas considered in this work is “wet gas,” which is mainly located in the southwest region of the Marcellus basin. For “dry gas,” the composition of which is almost pure methane, processing might be unnecessary.[14] Methane is the dominant component in the shale gas (75%−90% depending on the region), so the shale gas produced at the wellhead must be processed before it can be safely delivered to the high pressure, long-distance pipelines that transport the product to public consumers. The associated heavier hydrocarbons, including ethane, propane, butane, etc. that are known as natural gas liquids (NGLs), are usually taken as valuable by-products and can be sold separately.[44] It is worth noting that while the NGLs have substantially higher market value than natural gas, it is usually more cost-effective to use them as feedstocks to local petrochemical plants because of their high transportation costs. A typical design for a conventional shale gas processing plant includes the following processes: an acid gas removal process where acid impurities such as H_2S and CO_2 are removed; a sulfur recovery and tail gas cleanup processes where H_2S is converted to elemental sulfur; a dehydration process where water vapor is removed; a NGLs recovery process where NGLs are recovered from sales gas; a fractionation train that includes a series of distillation columns where different products from NGLs are further separated; and a nitrogen rejection process where the excess

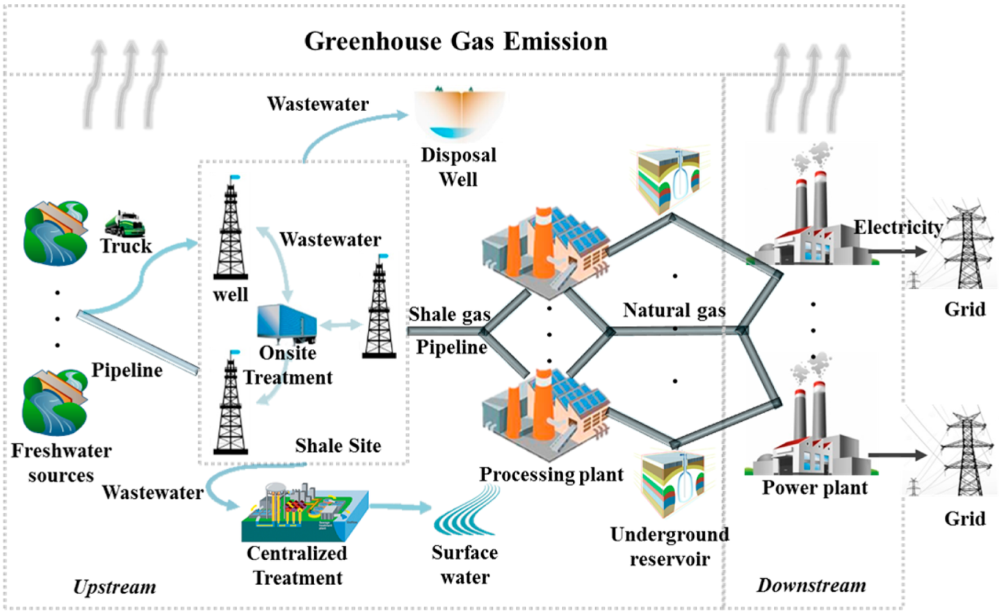


Figure 1. Superstructure of the shale gas supply chain.

nitrogen is rejected in the salable gas.[45−47] Because of the high capital investment of processing plants in the shale gas supply chain, the sizing and location of such processing plants are usually the most important decisions. The "pipeline-quality" natural gas from the processing plant can be directly transported to power plants for electric power generation. Alternatively, the processed gas can be transported to underground reservoirs and stored for an indefinite period of time. Underground reservoirs exist mainly for two reasons: (1) to accommodate fluctuations in demand, and (2) to accommodate fluctuations in price. There are three principle types of underground storage sites used in the United States today, namely, depleted natural gas or oil fields, aquifers, and salt caverns.[48] Water is transported through a set of transportation modes, such as truck or pipeline. All natural gas transportation is carried out with pipeline networks, the capacity and corresponding capital investment of which are important issues that need to be addressed.

A general shale gas supply chain superstructure is given in Figure 1. The following parameters are given: (1) capital investment cost functions regarding transportation of water, construction of processing plants, and installation of gas pipelines, (2) unit operating costs with respect to freshwater acquisition, well drilling, shale gas production, wastewater management, shale gas processing, storage of NGLs and natural gas, electricity generation, and transportation of water and gas, (3) capacity data related to freshwater supply, well drilling, different water management options, shale gas processing, NGLs storage, underground reservoir of natural gas, and different transportation modes, (4) unit GHG emissions data regarding freshwater acquisition, well drilling, hydraulic fracturing, completion, shale gas production, wastewater management, shale gas processing, storage, electricity generation, and all the transportation activities, and (5) problem specific data, including the shale gas production profile of each well, recovery factor of different onsite treatment technologies, composition of shale gas at each shale site, maximum number of wells that can be drilled at each shale site, efficiency of shale gas processing at the processing plant and electricity generation by natural gas at power plants.

The goal of this work is to maximize the economic and environmental performances of the shale gas supply chain network by optimizing the following strategic and operational decisions: (1) selection of freshwater sources and corresponding transportation modes, (2) drilling scheduling at each shale site, (3) wastewater management with regard to disposal wells, CWT, onsite treatment, and corresponding transportation modes, (4) location and sizing of processing plants, (5) selection of underground storage options as well as storage amounts for both NGLs and natural gas in each time period, and (6) installation and capacity of pipelines between shale sites, processing plants, underground reservoirs, and power plants.

In this work, a life cycle optimization framework is applied to overcome the drawbacks of classical LCA methodology.[49−51] The classical four-step, process-based LCA methodology is integrated with multiobjective optimization methods to provide design and operation alternatives as well as to identify the optimal decisions in terms of GHG emission. The domain of study is restricted to all life cycle stages from "well-to-wire" following the existing literature on shale gas LCA studies.[22−24] A 10-year lifetime of shale wells is assumed following the work of Hultman.[30] An additional sensitivity analysis of shale well lifetime is implemented, the results of which are given in the Supporting Information. Natural gas from Marcellus is considered as a fuel for electric power generation. Therefore, a functional unit of one Megawatt-hour (MWh) of electric power generated is employed following existing LCA work.[5,21,23,24] All descriptions provide a general statement of the shale gas supply chain design and operations problem. More detailed information can be found in the Supporting Information. In the following case study section, this general modeling framework is applied to a case study based on the Marcellus shale play with exact input data directly or indirectly derived from the literature.

MODEL FORMULATION AND GLOBAL OPTIMIZATION ALGORITHM

Model Formulation. According to the general problem statement in the previous section, a multiobjective, multiperiod MINLP model is developed to address the sustainable design and operations of shale gas supply chain networks, denoted as (P0). The detailed model formulation is provided in the Supporting Information.

$$\text{economic objective: min LC} = \frac{\text{TC}}{\text{TGE}} \text{ given in eq S63}$$

$$\text{environmental objective: min UE} = \frac{\text{TE}}{\text{TGE}} \text{ given in eq S81}$$

$$\begin{array}{lll} \text{P}(0) & \text{s.t.} & \text{mass balance constraints S1}-\text{S12} \\ & & \text{capacity constraints S13}-\text{S26} \\ & & \text{composition constraints S27} \\ & & \text{bounding constraints S28}-\text{S36} \\ & & \text{logic constraints S37}-\text{S41} \\ & & \text{economic constraints S42}-\text{S62} \\ & & \text{environmental constraints S64}-\text{S80} \end{array}$$

where LC denotes the levelized cost of electricity (LCOE), expressed as the total net present cost TC, divided by the total electricity generation TGE. UE denotes the GHG emissions corresponding to unit electricity power generation, expressed as the total GHG emission TE throughout the shale gas supply chain classified by the total amount of electricity generated TGE. The constraints are divided into five parts. (1) Mass balance constraints describe the relationship between the input and output streams of each unit within the supply chain network based on mass conservation of every species. (2) Capacity constraints describe the capacity limits of different activities in the shale gas supply chain, including freshwater acquisition, transportation, storage, gas processing, water management, market demand, etc. (3) Composition constraints specify water reuse for hydraulic fracturing. Treated wastewater will be blended with a certain percentage of freshwater to satisfy the reuse specification. (4) Bounding constraints are used to determine infrastructure construction and technology choice, namely pipeline construction, processing plant, water management options, etc. (5) Logic constraints describe the logical relationship of activities and basic assumptions, especially those regarding the drilling process. (6) Economic constraints calculate the total life cycle net present cost, including the negative terms accounting for the income from sales of NGLs, and positive terms regarding both capital investment as well as operation costs in the shale gas supply chain. (7) Environmental constraints calculate the total GHG footprint accounting for all activities from shale gas production to power generation.

In the following, the solution approach that is applied to tackle this multiobjective MINLP problem is briefly introduced.

Tailored Global Optimization Algorithm. The resulting problem is a nonlinear mixed-integer fractional programming (MIFP) problem, which is very challenging to solve and to obtain the optimal solution. Because of the nature of nonconvexity and the presence of integer variables, solving large-scale MIFP problems directly can be computationally intractable. Because none of the existing optimization software can return a feasible solution within a reasonable time, a tailored global optimization algorithm is developed to tackle this complex problem. We specifically implement the parametric algorithm to solve this nonlinear nonconvex MIFP problem, in which a parameter LC is introduced to replace the fractional objective function with a parametric function.[52−55] Consequently, Newton's method can be applied to search for the optimal value of LC, which equals the original optimal objective value. In each iteration of the parametric algorithm, though the fractional objective is circumvented, due to the nonlinear terms regarding capital investment, the resulting problem is still a nonconvex MINLP problem. Thus, we introduce the branch-and-refine algorithm based on successive piecewise linear approximations to tackle the remaining concave terms.[56−60] To provide a comprehensive idea of this algorithm, a pseudocode is presented in Table 1.

Table 1. Pseudocode of the Global Optimization Algorithm

```
global optimization algorithm
set LC = 0, $Iter^{out}$ = 1, Obj = +∞
while Obj ≥ $Tol^{out}$
    set LB = −∞, UB = +∞, $Iter^{in}$ = 1, Gap = +∞
    initialize with two insertion points
    while Gap ≥ $Tol^{in}$
        solve piecewise approximated problem, and obtain optimal solution $x^*$ and optimal objective function value $Obj^{lo}$
        evaluate the original objective function with $x^*$, and obtain $Obj^{up}$
        reconstruct relaxed problem by adding a new partition point
        set LB = max{LB, $Obj^{lo}$}, UB = min{UB, $Obj^{up}$}, Gap = |1 − LB/UB|, $Iter^{in}$ = $Iter^{in}$ + 1
    end while
    update LC = $\frac{TC^*}{TGE^*}$, $Iter^{out}$ = $Iter^{out}$ + 1
end while
return LC
```

By implementing this global optimization algorithm, the global optimization of the original nonconvex MIFP problem is transformed into a sequence of MILP subproblems. The details of this algorithm are given in the Supporting Information.

CASE STUDY AND RESULTS DISCUSSION

To illustrate the application of the proposed model and solution approaches, two case studies are given. A smaller one for a simplified supply chain optimization problem is presented mainly to verify the proposed solution approach. Details on this case study are included in the Supporting Information. A larger case study is given in this section. Because regional differences can significantly affect the optimal technology selection and design decisions of shale gas supply chains, one specific case study based on the Marcellus shale play in southwest PA is considered in this work. A detailed description of this problem is given below. It is worth noting that the proposed model and solution methods are general enough, so the application of the proposed modeling framework and optimization algorithm is not limited to any specific region.

In this large scale case study, 3 freshwater sources are considered, and the freshwater withdrawal availability of each is estimated based on historical flow rates in the Marcellus shale play with consideration of seasonal fluctuations.[13,61] Three shale sites are included, and each can drill up to 4 to 8 wells at maximum.[62] The whole process from well drilling to well completion takes roughly three months,[14] corresponding to 1 time period in this model. Drilling activities are confined to the first 3 years. An exponentially decreasing approximation of the shale gas production profile is considered, given as a function of time depicted in Figure S6 in Supporting Information.[14] Drilling water demand is assumed to be dependent on the number of wells drilled. Produced water is assumed proportional to the amount of shale gas produced.[40,63] There are 5 Class II disposal wells,[64] 3 commercial CWT facilities,[65] and 3 types of onsite desalination technologies, namely MSF, MED, and RO.[66,67] There are 2 potential conventional shale gas processing plants,[46] 2 depleted natural gas fields as underground storage sites,[48] and 2 Gas Turbine Combined Cycle (GTCC) power plants with 50% generation efficiency based on LHV.[27,68] The total planning horizon is 10 years, which is close to the real productive life of Marcellus wells, divided into 40 time periods, i.e. one-quarter per time period.[14,69] All detailed input data are based on existing literature and provided in the Supporting Information. It is worth noting that due to the development of performance standards and regulation standards, some of the assumptions applied in the data sources, regarding drilling, production, storage, transportation, infrastructures et al., might not be suitable for the latest practices. Besides, the corresponding GHG emissions could be reduced because of these recent practices. Nevertheless, the proposed modeling framework and solution methods are general enough that can be easily adapted to these updates. The resulting problem has 5028 continuous variables, 203 discrete variables, and 6907 constraints. All of the models and solution procedures are coded in GAMS 24.4.1[70] on a PC with Intel Core i5-2400 CPU @ 3.10 GHz and 8.00 GB RAM, running Windows 8, 64-bit operating system. Furthermore, the MILP problems are solved using CPLEX 12.6. The MINLP solvers utilized include global optimizers SCIP 3[71] and BARON 14.[72] The absolute optimality tolerance for all solvers is set to 0. The optimality tolerance tol for the inner loop in the proposed global optimization method is set to 10^{-2}, and δ for the outer loop is set to 10^{-2}. Detailed computational performance data are provided in the Supporting Information.

Pareto-Optimal Curve. The resulting MINLP problem is solved using the global optimization algorithm proposed in Section 3 and 10 Pareto optimal solutions are obtained, which form the Pareto-optimal curve shown in Figure 2. The *x*-axis represents the GHG emissions corresponding to unit electricity generation. The *y*-axis represents the levelized cost of electricity. The levelized cost of electricity decreases as the GHG emission increases, which explicitly shows the trade-off between the economic and environmental objectives. The region above the Pareto-optimal curve is the suboptimal region, and the region below the curve is the infeasible region.

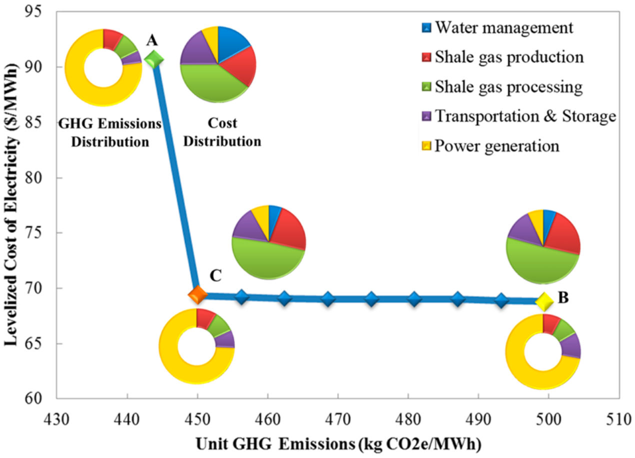


Figure 2. Pareto-optimal curve of the case study with breakdown of the cost and emissions: pie charts represent cost breakdowns; the donut charts represent emissions breakdowns.

As can be seen in Figure 2, the extreme point A has the lowest GHG emissions per unit electricity generated of 443 kg CO_2e/MWh, and it has the highest levelized cost of electricity of $69/MWh. On the contrary, point B has the lowest levelized cost of electricity of $69/MWh and the highest GHG emissions per unit electricity generated of 499 kg CO_2e/MWh. Solutions between points A and B have lower levelized costs of electricity than A and lower GHG emissions than B. Point C is the recommended point, which is characterized by both economic efficiency and environmental sustainability. The levelized cost of electricity of point C is $69/MWh and the unit GHG emissions is 450 kg CO2e/MWh.

By reviewing related literature, we note that the U.S. Energy Information Administration (EIA) reports a regional variation in LCOE for natural gas-fired electricity from $61 to $76/MWh.[73] According to the work by Heath et al.,[28] recent results on life cycle GHG emissions of shale gas for electricity generation range from around 440 to 760 kg CO_2e/MWh. We present a detailed comparison of these results in Figure 3. In general, the result obtained in this work is within the same ranges of other LCA studies. When focusing on the specific LCA results of Marcellus shale play, the recommended point C in this work, while maintaining close economic efficiency to point B, has lower GHG emissions. It is 7% lower than the result reported by Jiang et al, and 3% lower than that reported by Laurenzi and Jersey. Though a relatively small change in unit GHG emissions is observed, a significant reduction in total GHG emissions can be achieved considering the amount of natural gas consumed to generate electricity. Our model and input data are further validated by comparing these published results.

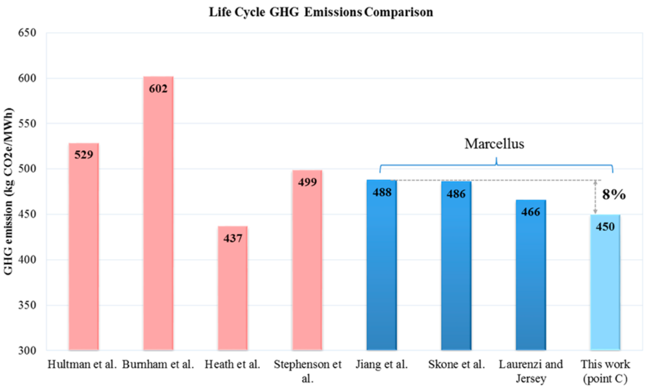
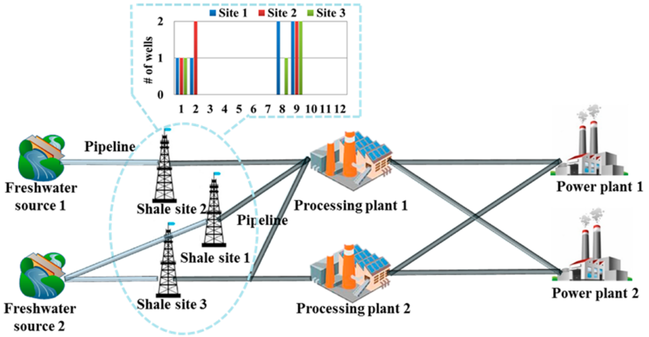
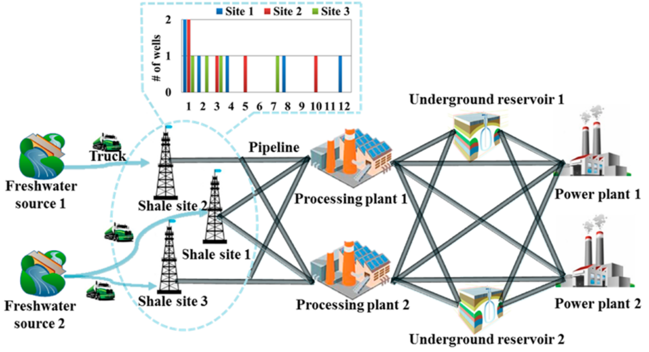


Figure 3. Comparison of results regarding life cycle GHG emissions from electricity generated using shale gas.[17,21,22,24,28,30,74]

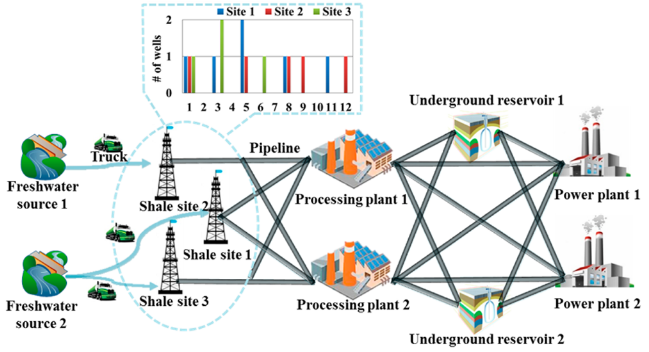
In Figure 2, the detailed GHG emissions breakdown and corresponding cost breakdown of the three mentioned points are also provided. As can be seen, all three points have similar GHG emissions breakdowns. Power generation is identified as the primary source of GHG emissions, the percentage of which ranges from 76% for point A to 72% for point B. This result is reasonable and similar to results reported by other LCA studies, as in this model, all of the produced natural gas is burned at the power plants with a conventional combined cycle, where significant GHG emissions are generated.[24,27] Shale gas production, processing, and transportation and storage account for the remaining GHG emissions. These GHG emissions are mainly caused by related energy consumption, venting activities, and other losses. Compared with the processes directly related to shale gas production, the GHG emissions in water management processes, including freshwater acquisition, wastewater treatment, and corresponding transportation are



(a) Shale gas supply chain strategies of point A



(b) Shale gas supply chain strategies of point B



(c) Shale gas supply chain strategies of point C

Figure 4. Shale gas supply chain strategies comparison among (a) point A, (b) point B, and (c) point C.

negligible. Meanwhile, we note that a higher cost is observed in point A, where roughly 17% of the total cost is from water management, higher than point B and point C. In point A, because the only objective is to minimize the unit GHG emissions, pipelines are widely used to transport freshwater, resulting in a high capital investment. Cost breakdowns for points B and C are similar, where shale gas processing accounts for about 50% (51% for point B and 49% for point C) of the total cost. Other major costs include shale gas production (23% for point B and 23% for point C), transportation and storage (14% for point B and 15% for point C), and power generation (7% for point B and 8% for point C).

Trade-off between Economic and Environmental Performance. In this section, the comparison between the two extreme points A and B as well as the recommended point C is presented within the context of economic and environmental criteria. Decisions regarding the supply chain network, drilling schedule, water management, and production profile are fully reviewed and discussed.

First, the detailed production profile and decision parameters are summarized as follows. For point A, a total of 2.40 billion standard cubic feet (bscf) of shale gas is produced, with a total freshwater consumption of 125 944 barrels. Both processing plants are built with capacities of 100 million standard cubic feet (mmscf) of shale gas per quarter. A total of 260 394 MWh of electricity is generated. For point B, 2.49 bscf of shale gas is produced, and the total freshwater consumption is 128 534 barrels. Two processing plants are built with capacities of 30 mmscf shale gas per quarter and 56 shale gas mmscf per quarter, respectively. A total of 268 971 MWh of electricity is generated. Point C is identified with an intermediate result: 2.43 bscf shale gas is produced, with 126 140 barrels freshwater consumed. Two processing plants are built with capacities of 30 mmscf per quarter and 63 mmscf per quarter, respectively. The total electricity generation is 262 429 MWh.

Supply Chain Network. As shown in Figure 4, the supply chain network structures of all three points have the same freshwater supply strategy. The significant differences regarding the network among the two extreme points A and B as well as the recommended point C include: (1) Freshwater transportation. Pipelines appear to be a preferable option for transporting freshwater to shale sites when minimizing the unit GHG emission in point A. However, for both point B and point C, using trucks to transport freshwater results in improved economic performance. (2) Pipeline network. Between the shale sites and processing plants there exist more pipeline connections for point B and point C, providing more flexibility for shale gas processing activities. However, for point A, such a network is simpler so as to reduce unnecessary GHG emissions. (3) Underground reservoir. In the network of point A, underground reservoirs are not utilized, which means all of the processed natural gas will be directly transported to power plants for electricity generation. As a result, emissions from storage and transportation activities of sales gas are avoided. Meanwhile, for both point B and point C, underground reservoirs are used as important "buffers," coordinating the drilling activities and market demand, thus reducing the overall cost in this shale gas supply chain.

Drilling Strategy. As can be seen in Figure 3, points A, B, and C return significantly different drilling strategies. For point A minimizing the unit GHG emissions, almost half of the wells are drilled in the beginning to satisfy the necessary demand of markets, and the remaining wells are postponed to later times (around period 8 and 9). Meanwhile, for point B minimizing the LCOE, drilling activities tend to be evenly distributed. More shale wells are drilled in the beginning. Considering the exponentially decreasing shale gas production profile for each well, additional wells drilled in later times could compensate for this decrease such that the overall shale gas production maintains a relatively steady value. As a result, the corresponding facilities can be designed with a more suitable capacity, reducing the capital investment. Meanwhile, a steady shale gas production profile would give the whole shale gas supply chain more options for improving economic performance. As expected, the recommended point C applied a similar strategy to point B in that wells are evenly drilled throughout the first three years. To convey more clearly the shale gas production comparisons among these scenarios, the following production profiles comparison is presented.

In Figure 5, a "density map" is presented, where the colors range from white to blue, corresponding to the smallest and largest production values for each time period, respectively.

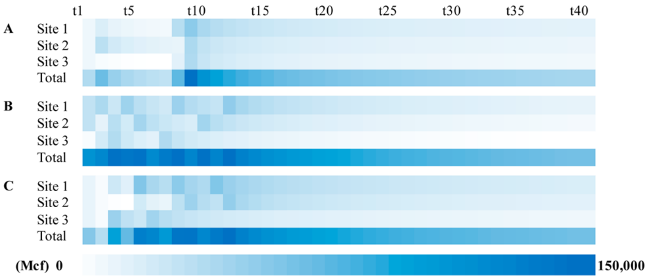


Figure 5. Shale gas production profile of point A, point B, and point C.

Because the drilling process requires lead time, assumed to be 1 quarter in this model,[14] the shale gas production is 0 in the first quarter. Point A has relatively lower shale gas production at first, and a production peak occurs around quarter 9. Point B maintains a stable production profile mainly due to its aforementioned drilling strategy. The production profile of point C is a sort of combination of points A and B, where increased shale gas production can be observed near quarter 10, when more wells are drilled.

Water Management Strategy. These three points adopt different transportation modes for freshwater acquisition. As mentioned above, because the objective of point A is to minimize the unit GHG emissions, pipelines are proved to be more competitive than trucks, resulting in less GHG emissions. For point B and point C, trucks are a more economical and flexible transportation option for freshwater due to the high capital investment of pipeline construction. Regarding the wastewater management, three options are considered, namely disposal wells, CWT, and onsite treatment. In addition, three onsite treatment technologies are considered in the case study, including MSF, MED, and RO (Figure 6). The unit treatment costs and emission data are summarized in Table 2.

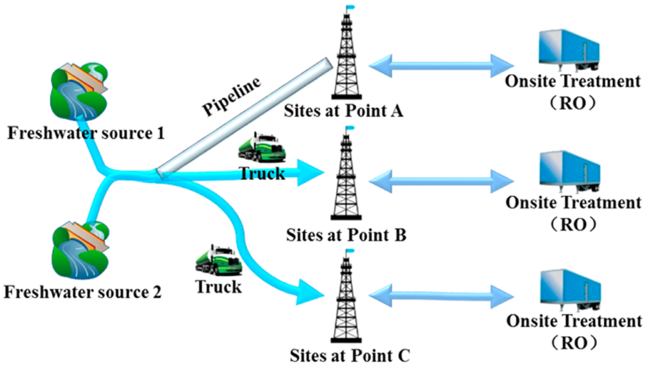


Figure 6. Water management strategy summary of points A, B, and C.

According to the optimal results, all three points choose onsite treatment with RO technology as the only way to treatment wastewater. Compared with other options and technologies, RO has significantly lower unit GHG emissions. Although the unit cost is lower than other onsite treatment technologies including MSF and MED, it is still higher than underground disposal and CWT. RO technology usually has a smaller treatment capacity compared to MSF and MED. However, the extra transportation costs required for underground disposal and CWT make RO economically competitive. This explains why all three points with different objectives choose RO as the wastewater management option. These results are consistent with the trend reported by Wilson and VanBriesen[42] in that the application of onsite treatment has grown rapidly as the primary option of wastewater management in the Marcellus shale play. Moreover, by reviewing the recently released performance standards and regulatory standards by Center for Sustainable Shale Development (CSSD),[76] we note that a minimum of 90% of the flowback and produced water is required to be recycled, and multiple regulations with respect to reducing emissions of flaring, venting, drilling, fracturing, storage, transportation et al. are implemented. These performance standards not only validate some of the conclusions (e.g., wide application of onsite treatment and reuse), but predict a further reduction of GHG emission of shale gas supply chain.

Table 2. Economic and Environmental Comparison between Water Management Options

options	unit cost ($/barrel water)	ref	unit emission (g CO_2 e/barrel water)	ref
underground disposal	1.0−1.4	40	1000−1040	18
CWT	3.2−3.8	40	1260−1300	75
onsite treatment (MSF)	6.5	66	3797	66, 67
onsite treatment (MED)	5.4	66	2813	66, 67
onsite treatment (RO)	4.7	66	350	66, 67

To give a comprehensive comparison among extreme points A and B as well as recommended point C, Figure 7 is presented to illustrate the solution results regarding total shale gas production, total revenue, total GHG emission, total power generation, and total water consumption. Due to the different order of magnitude in terms of different dimensions, we set the value of point C as the reference with value 1 and use the ratio instead of the exact values for points A and B.

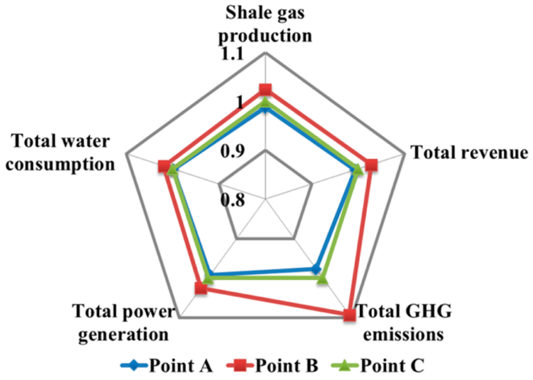


Figure 7. Comprehensive comparison among points A, B, and C.

As can be seen, the best economic performance can be obtained by point B. Point A has lower GHG emissions with similar shale gas production, water consumption, and electricity generation. Point C has close economic performance to point B; meanwhile, it maintains a reasonable GHG emissions level.

In this work, we proposed a multiobjective MINLP model for the sustainable design and operations of shale gas supply chain networks. A cooperative system is assumed throughout the life cycle. Through a series of comprehensive comparison and discussion, we conclude that improved economic performance can be achieved by using trucks to transport freshwater, maintaining a stable shale gas production profile (meaning evenly distributed drilling activities), introducing more transportation links, and taking advantage of underground reservoirs as "buffers" in the supply chain. Meanwhile, to pursue a more environmentally friendly outcome, drilling activities should be more concentrated, unnecessary transportation links should be avoided, pipelines should be used to transport freshwater, and unnecessary gas storage is to be avoided. Managing wastewater with RO technology onsite is identified as the best wastewater treatment option with excellent economic and environmental performance. In the future work, more options such as multiple end consumptions of natural gas and carbon capture and storage can be integrated in this shale gas supply chain, and consideration of uncertainty can be included to achieve more accurate solutions.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

Background information, detailed model formulation, computational case study and corresponding performance, sensitivity analysis, input data, and nomenclature are included. The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acssuschemeng.5b00122.

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Notes

The authors declare no competing financial interest.

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