Supporting Information

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

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Background Information

In this section, a brief introduction is given on the life cycle optimization framework applied in this work.

Life Cycle Optimization

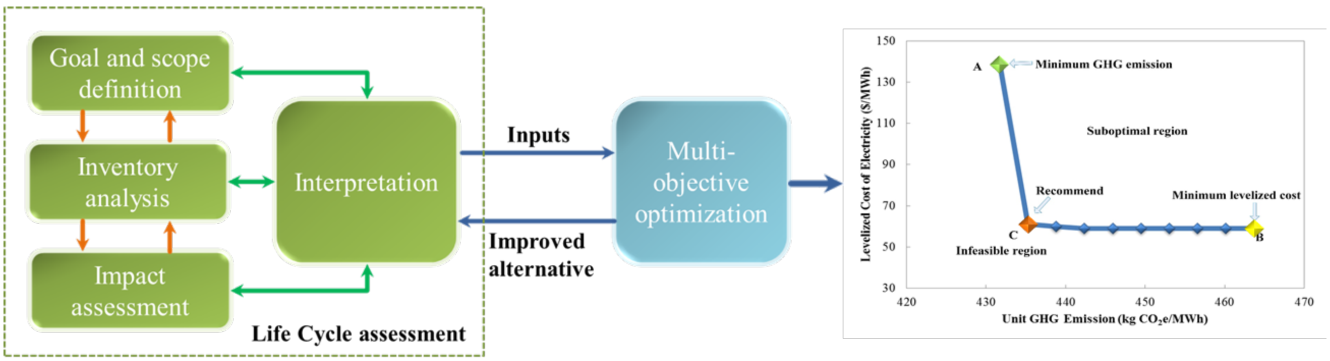

Figure S1. Life cycle optimization modeling framework

In this work, a life cycle optimization framework is applied, which integrates the classical four-step process-based LCA methodology with the multiobjective optimization method. It provides design and operation alternatives as well as identifying the optimal decisions in terms of environmental performance.[1-3] The framework of the life cycle optimization can be illustrated by Figure S1. The main information regarding the LCA of this shale gas supply chain networks is presented as follows.

Goal and Scope Definition

The primary goal of this study is to identify the most sustainable shale gas supply chain network from the production of shale gas at shale sites to the electricity generation at power plants. While GHG emissions from the upstream component of the shale gas supply chain may be significant, they must be placed into context of the overall life cycle of shale gas, which in most cases ends in combustion for power generation.[4] In this work, the domain of study is restricted to all life cycle stages from “well-to-wire” following the existing literature on shale gas LCA studies.[5-7] As shown in Figure S2, the whole system of the shale gas life cycle can be taken as an integration of shale gas supply chain and water supply chain. There are commonly three parts of the supply chain, including the “upstream”, “midstream”, and “downstream”. However, in this work. the system is divided into two sections, including the “upstream” section and the “downstream” section following the work by Laurenzi & Jersey.[5] The “upstream” section involves all the phases of the shale gas life cycle preceding the power plant, including well pad preparation, well drilling, hydraulic fracturing, well completion, water management, shale gas production, processing, and storage. Due to unreliable assumptions and limited data on shale well workovers, this activity is not considered in this work.[5, 8] The "downstream" section mainly involves power generation. All the aforementioned processes and activities within this system boundary not only have economic impacts on this system, but also generate GHG emissions, bringing about environmental impacts. In this work, a 10-year shale well lifetime is assumed following the work of Hultman.[9] According to EIA data, the half-life of a shale well is about 30 months, so roughly 95% of the estimated ultimate recovery (EUR) of a shale well will have been depleted after ten years. Moreover, as reported by the Real Marcellus Gas Production, there is an approximately 65% drop in production over the first 3 years, with further declines of 8% per year after that.[10] Therefore, the 10-year lifetime assumption is reasonable here.

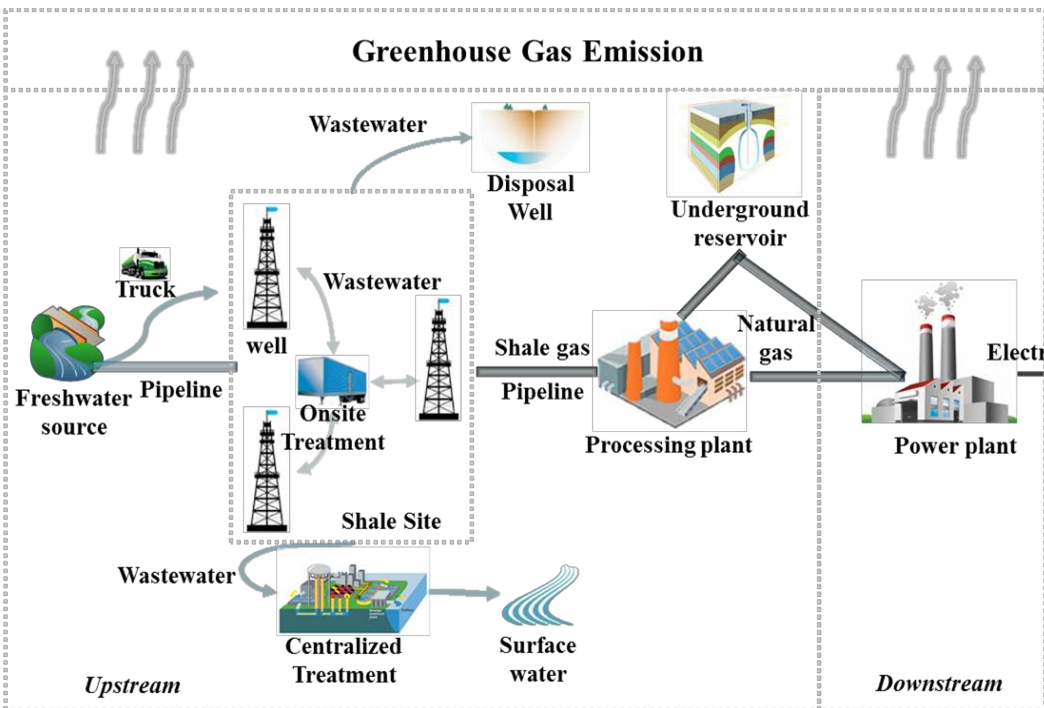

Figure S2. Illustration of general shale gas supply chain networks

According to the International Organization for Standardization (ISO), classical LCAs must report environmental impacts in terms of a "functional unit" for a better comparison of impacts associated with alternative products. In this work, natural gas from the Marcellus shale play is considered as a fuel for electric power generation. As one of the most important usages of natural gas in the U.S., electric power generation is widely considered in LCA studies as the end use destination of natural gas.[5, 7, 11] Therefore, a functional unit of one MWh of electric power generated at the power plant is employed following existing LCA work.[5, 7, 12] All the economic input data used in this work are directly or indirectly derived from the literature.[13-16] All of the LCA data are derived from reviewing existing LCA studies of shale gas, especially those of the Marcellus shale play.

Inventory Analysis

The life cycle inventory is analyzed regarding processes/activities in the life cycle stages within the predefined system boundary. The most relevant inputs/outputs of materials and energy use associated with corresponding activities can be identified and quantified based on the mass balance as well as the energy balance. The inventory mentioned here is different from the concept generally applied in supply chain study, and the inventory data regarding processes/activities are actually decision variables to be optimized in this shale gas supply chain network. By conducting an inventory analysis, it is possible to quantify the impacts and make decisions accordingly.

Impact Assessment

In this work, GHG emissions are quantified in units of CO_2-equivalent, which is a metric that compares the radiative forcing associated with a GHG relative to that of CO_2. To be more specific, the 100-year global warming potentials (GWP) (25 g CO_2/ g CH_4) is utilized to assess the environmental impacts of different GHGs.[17] With the predefined functional unit, the environmental impact is evaluated based on GHG emissions per unit electricity generation as kg CO_2e/MWh.

Interpretation

LCA results are analyzed to provide criteria and quantitative measurements for comparison of different supply chain design and operation alternatives. In this work, the optimization tool and environmental impacts assessment are coupled together to provide a systematic approach for generating alternatives and identifying the optimal decision in terms of environmental performance. By solving the resulting multi-objective optimization problem, the Pareto-optimal frontier can be obtained consisting of a set of Pareto-optimal solutions, which reveals the trade-off between the economic objective as well as the environmental objective, and helps develop a more sustainable shale gas supply chain network.

Model Formulation and Solution Method

The mathematical model for the optimization of design and operations of shale gas supply chain is a mixed-integer nonlinear program. The general formulation is provided in the main text. Here we present the detailed description of all the constraints as well as objective functions. All the parameters are denoted with lower-case symbols, and all of the variables are denoted with upper-case symbols.

Constraints

Mass Balance Constraints

The total water supply at each shale site should be satisfied by freshwater from water sources and reused water from onsite treatment.

$$\sum_{s\in S}\sum_{k\in K} FW_{s,i,k,t} + \sum_{o\in O} lo_o \cdot WTO_{i,o,t} = FDW_{i,t},\ \forall i,\ t \tag{S1}$$

where $FW_{s,i,k,t}$ denotes the amount of freshwater acquired from freshwater source s at shale site i using transportation mode k in time period t. The second term denotes the water reused from onsite treatment. lo_o denotes the recovery factor for treating wastewater by onsite treatment technology o. $WTO_{i,o,t}$ denotes the amount of wastewater treated by onsite treatment technology o at shale site i in time period t. $FDW_{i,t}$ is the demand of freshwater at shale site i in time period t.

The amount of freshwater required at each shale site in each time period equals the summation of water usage for drilling and hydraulic fracturing, where the drilling water usage is proportional to the number of wells being drilled, and the hydraulic fracturing water usage is proportional to the amount of wastewater produced at shale site i. This relationship is given by:

$$FDW_{i,t} = {WP_{i,t}}/{wrf_i} + wd_i \cdot NN_{i,t},\ \forall i,\ t \tag{S2}$$

where $WP_{i,t}$ denotes the wastewater production rate during fracking process at shale site i in time period t. wrf_i is the recovery ratio of water for hydraulic fracturing process at shale site i. wd_i denotes the average drilling water usage at shale site i. $NN_{i,t}$ stands for the number of wells drilled at shale site i in time period t.

The wastewater production rate during the fracking process is proportional to the total shale gas production rate at a shale site,[18]

$$WP_{i,t} = cc_i \cdot SP_{i,t},\ \forall i,\ t \tag{S3}$$

where cc_i is the correlation coefficient for shale gas production and wastewater production of a shale well at shale site i, $SP_{i,t}$ is the shale gas production rate at shale site i in time period t.

At each shale site, the total amount of produced wastewater, including the wastewater from drilling and hydraulic fracturing, should equal to the total water flow with respect to different water management options, including CWT, disposal, onsite treatment, and onsite storage.

$$WP_{i,t} + wd_i \cdot wrd_i \cdot NN_{i,t} = \sum_{c\in C}\sum_{k\in K} WTC_{i,c,k,t} + \sum_{d\in D}\sum_{k\in K} WTD_{i,d,k,t} + \sum_{o\in O} WTO_{i,o,t},\ \forall i,\ t \tag{S4}$$

where wrd_i denotes the recovery ratio for drilling process at shale site i. $WTC_{i,c,k,t}$ and $WTD_{i,d,k,t}$ denotes the amount of wastewater transported with transportation mode k in time period t from shale site i to CWT facility c and disposal well d, respectively.

The total shale gas production rate at a shale site equals the sum of that of different wells. Note that τ is the age of shale well such that $\tau = t - t'$, and t' is the time period when this well is drilled. The total shale gas production at each shale site in each time period can be calculated by:

$$SP_{i,t} = \sum_{t'=1}^{t-1} NN_{i,t'} \cdot spp_{i,t-t'}, \ \forall i, \ t \geq 2 \tag{S5}$$

where $spp_{i,t-t'}$ denotes the shale gas production profile of a shale well drilled at time period t' at shale site i in time period t. Therefore the age of this well would be $t- t'$, and we use this time-dependent parameter to describe the decreasing feature of the shale gas production profile of a certain well as shown in Figure 3 in the main text.

The total amount of shale gas production at each shale site should equal the total amount of shale gas transported to different processing plants,

$$SP_{i,t} = \sum_{p \in P} STP_{i,p,t}, \ \forall i, \ t \tag{S6}$$

where $STP_{i,p,t}$ denotes the amount of shale gas transported from shale site i to processing plant p in time period t.

The total methane produced at a processing plant should equal the methane composition of the total shale gas transported from different shale sites taking into account processing efficiency. The amount of NGLs produced at a processing plant is determined by similar equations.

$$\sum_{i \in I} STP_{i,p,t} \cdot pef \cdot mc_i = SPM_{p,t}, \ \forall p, \ t \tag{S7}$$

$$\sum_{i \in I} STP_{i,p,t} \cdot pef \cdot lc_i = SPL_{p,t}, \ \forall p, \ t \tag{S8}$$

where pef is the processing efficiency in terms of raw shale gas. mc_i denotes the average methane composition in shale gas at shale site i. $SPM_{p,t}$ is the amount of natural gas produced at processing plant p in time period t. lc_i is the average NGLs composition in shale gas at site i. $SPL_{p,t}$ stands for the amount of NGLs produced at processing plant p in time period t.

The amount of NGLs produced, to be stored and sold at each processing plant should satisfy the following mass balance relationship,

$$SPL_{p,t} + SPS_{p,t-1} = PLS_{p,t} + SPS_{p,t}, \ \forall p, \ t \geq 2 \tag{S9}$$

where $SPS_{p,t}$ denotes the amount of NGLs stored at processing plant p in time period t. $PLS_{p,t}$ denotes the amount of NGLs sold at processing plant p in time period t.

The total amount of natural gas produced at a processing plant should equal the summation of natural gas transported from the processing plant to different power plants and underground reservoirs.

$$SPM_{p,t} = \sum_{m\in M} STPM_{p,m,t} + \sum_{u\in U} STPU_{p,u,t}, \ \forall p, \ t \qquad \text{(S10)}$$

where $STPM_{p,m,t}$ denotes the amount of natural gas transported from processing plant p to power plant m in time period t. $STPU_{p,u,t}$ denotes the amount of natural gas transported from processing plant p to underground reservoir u in time period t.

For natural gas at each underground reservoir, the following input-output mass balance relationship should be satisfied,

$$\sum_{p\in P} STPU_{p,u,t} + URS_{u,t-1} = \sum_{m\in M} STUM_{u,m,t} + URS_{u,t}, \ \forall u, \ t \geq 2 \qquad \text{(S11)}$$

where $URS_{u,t}$ denotes the amount of natural gas stored at underground reservoir u in time period t. $STUM_{u,m,t}$ denotes the amount of natural gas transported from underground reservoir u to power plant m in time period t.

The total amount of electricity generation at power plant m in each time period is proportional to the amount of natural gas transported from processing plants and underground reservoirs to the power plant.

$$GE_{m,t} = ue \cdot \left(\sum_{p\in P} STPM_{p,m,t} + \sum_{u\in U} STUM_{u,m,t} \right), \ \forall m, \ t \qquad \text{(S12)}$$

where ue denotes the amount of electricity generated per unit shale gas input. We note that we have already considered the power generation efficiency from natural gas, which is 50% based on LHV integrated in this parameter.[4] $GE_{m,t}$ denotes the amount of electricity generated at power plant m in time period t.

Capacity Constraints

The total freshwater supply from each freshwater source to all the shale sites by different transportation modes should not exceed the supply capacity of this freshwater source, given by:

$$\sum_{i\in I} \sum_{k\in K} FW_{s,i,k,t} \leq fca_{s,t}, \ \forall s, \ t \qquad \text{(S13)}$$

where $fca_{s,t}$ denotes the freshwater supply capacity at freshwater source s in time period t.

The amount of shale gas transported by pipeline from shale site i to processing plant p is bounded by the capacity of pipelines, given by:

$$STP_{i,p,t} \leq TCP_{i,p}, \ \forall i, \ p, t \qquad \text{(S14)}$$

where $TCP_{i,p}$ denotes the capacity of pipeline from shale site i to processing plant p.

The amount of NGLs stored at processing plant cannot exceed its storage capacity, given by:

$$SPS_{p,t} \le psc_p \cdot YP_p, \ \forall p, \ t \tag{S15}$$

where psc_p denotes the storage capacity of NGLs for each time period at processing plant p. YP_p are binary variable that equals to 1 if processing plant p is set up

The amount of natural gas transported by pipeline is bounded by the capacity of pipelines, including pipelines from processing plant p to power plant m, from processing plant p to underground reservoir u, and from underground reservoir u to power plant m, given by the following constraints, respectively:

$$STPM_{p,m,t} \le TCPM_{p,m}, \ \forall p, \ m, t \tag{S16}$$

$$STPU_{p,u,t} \le TCPU_{p,u}, \ \forall p, \ u, t \tag{S17}$$

$$STUM_{u,m,t} \le TCUM_{u,m}, \ \forall u, \ m, t \tag{S18}$$

where $TCPM_{p,m}$, $TCPU_{p,u}$, $TCUM_{u,m}$ denote the pipeline capacity from processing plant p to power plant m, from processing plant p to underground reservoir u, and from underground reservoir u to power plant m, respectively.

The total amount of wastewater from different shale sites transported by different transportation modes and treated by each CWT facility cannot exceed its capacity,

$$\sum_{i \in I} \sum_{k \in K} WTC_{i,c,k,t} \le cca_{c,t}, \ \forall c, \ t \tag{S19}$$

where $cca_{c,t}$ denotes the capacity for wastewater treatment at CWT facility c in time period t.

The total amount of wastewater from all the shale sites handled by each disposal well should not exceed its disposal capacity,

$$\sum_{i \in I} \sum_{k \in K} WTD_{i,d,k,t} \le dca_{d,t}, \ \forall d, \ t \tag{S20}$$

where $dca_{d,t}$ denotes the capacity for underground injection at disposal well d in time period t.

The total amount of shale gas from all the shale sites processed by each processing plant should not exceed its processing capacity,

$$\sum_{i \in I} STP_{i,p,t} \le PC_p, \ \forall p, \ t \tag{S21}$$

where PC_p denotes the capacity of processing plant p.

The total amount of natural gas stored at underground reservoir cannot exceed its working gas capacity, given by:

$$URS_{u,t} \le uca_u,\ \forall u,\ t \tag{S22}$$

where uca_u denotes the working gas capacity of underground reservoir *u*.

The amount of natural gas injected in each underground reservoir cannot exceed its injection capability for each time period,

$$\sum_{p \in P} STPU_{p,u,t} \le uic_u,\ \forall u,\ t \tag{S23}$$

where uic_u denotes the injection capacity for each time period of underground reservoir *u*.

The amount of natural gas withdrawn from each underground reservoir is bounded by its withdrawal capability for each time period, given by:

$$\sum_{m \in M} STUM_{u,m,t} \le uwc_u,\ \forall u,\ t \tag{S24}$$

where uwc_u denotes withdrawal capacity for each time period of underground reservoir *u*.

The total amount of natural gas transported from all the processing plants and underground reservoirs to each power plant must stay within its demand bound,

$$dm_{m,t} \le \sum_{p \in P} STPM_{p,m,t} + \sum_{u \in U} STUM_{u,m,t} \le dmup_{m,t},\ \forall m,\ t \tag{S25}$$

where $dm_{m,t}$ denotes the minimum demand of natural gas at power plant *m* in time period *t*. $dmup_{m,t}$ denotes the maximum demand of natural gas at power plant *m* in time period *t*.

The total amount of NGLs sold at all of the processing plants is also constrained by the demand of NGLs,

$$dl_t \le \sum_{p \in P} PLS_{p,t} \le dlup_t,\ \forall t \tag{S26}$$

where dl_t denotes the minimum demand for NGLs in time period *t*. $dlup_t$ denotes the maximum demand for NGLs in time period *t*.

Composition Constraints

In order to satisfy the reuse specification for hydraulic fracturing, the blending ratio of freshwater to treated water from onsite treatment must be greater than a certain value, given by,

$$\sum_{o \in O} rf_o \cdot lo_o \cdot WTO_{i,o,t} \le \sum_{s \in S} \sum_{k \in K} FW_{s,i,k,t},\ \forall i,\ t \tag{S27}$$

where rf_o denotes the ratio of freshwater to wastewater required for blending after treatment by technology *o*.

Bounding Constraints

If transportation mode *k* is installed from freshwater source *s* to shale site *i*, the amount of freshwater transported by transportation mode *k* is constrained by its capacity; otherwise, the amount of freshwater transported by transportation mode *k* should equal zero. Thus, we have the following constraints,

$$FW_{s,i,k,t} \le tsc_{s,i,k} \cdot XS_{s,i,k}, \ \forall s, \ i, \ k, t \tag{S28}$$

where $tsc_{s,i,k}$ denotes the transportation capacity for transportation mode *k* from source *s* to shale site *i*. $XS_{s,i,k}$ is a binary variable that equals 1 if transportation mode *k* is chosen to transport freshwater from source *s* to shale site *i*.

If transportation mode *k* is installed from shale site *i* to CWT facility *c*, the amount of wastewater transported by transportation mode *k* cannot exceed its capacity; otherwise, it equals zero.

$$WTC_{i,c,k,t} \le tcc_{i,c,k} \cdot XC_{i,c,k}, \ \forall i, \ c, \ k, t \tag{S29}$$

where $tcc_{i,c,k}$ denotes the transportation capacity for transportation mode *k* from shale site *i* to CWT facility *c*. $XC_{i,c,k}$ is a binary variable that equals 1 if transportation mode *k* is chosen to transport wastewater from shale site *i* to CWT facility *c*.

If transportation mode *k* is installed from shale site *i* to disposal well *d*, the amount of wastewater transported by transportation mode *k* is bounded by its capacity; otherwise, it equals zero.

$$WTD_{i,d,k,t} \le tdc_{i,d,k} \cdot XD_{i,d,k}, \ \forall i, \ d, \ k, t \tag{S30}$$

where $tdc_{i,d,k}$ denotes the transportation capacity for transportation mode *k* from shale site *i* to disposal well *d*. $XD_{i,d,k}$ is a binary variable that equals to 1 if transportation mode *k* is chosen to transport wastewater from shale site *i* to disposal well *d*.

If a certain onsite treatment technology is applied at a shale site, the amount of wastewater treated onsite should be bounded by its capacity; otherwise, the amount of wastewater treated onsite should be zero. This relationship can be modeled by the following inequality,

$$ocl_o \cdot YO_{i,o} \le WTO_{i,o,t} \le ocu_o \cdot YO_{i,o}, \ \forall i, \ o, \ t \tag{S31}$$

where ocl_o denotes the minimum treatment capacity for onsite treatment technology *o*. ocu_o denotes the maximum treatment capacity for onsite treatment technology *o*. $YO_{i,o}$ is a binary variables that equals 1 if onsite treatment technology *o* is applied at shale site *i*.

The constraints for the capacity of pipeline transporting shale gas from shale site *i* to processing plant *p* are given by,

$$tpcl \cdot XP_{i,p} \le TCP_{i,p} \le tpcu \cdot XP_{i,p}, \ \forall i, \ p \tag{S32}$$

where *tpcl* and *tpcu* stand for the minimum and the maximum capacity of pipeline transporting shale gas, respectively. $XP_{i,p}$ is a binary variable that equals 1 if pipeline is installed to transport shale gas from shale site *i* to processing plant *p*.

Similarly, the constraints for the capacity of all the pipelines transporting natural gas are given by,

$$tmcl \cdot XPM_{p,m} \le TCPM_{p,m} \le tmcu \cdot XPM_{p,m}, \ \forall p, \ m \tag{S33}$$

$$tmcl \cdot XPU_{p,u} \le TCPU_{p,u} \le tmcu \cdot XPU_{p,u}, \ \forall p, \ u \tag{S34}$$

$$tmcl \cdot XUM_{u,m} \le TCUM_{u,m} \le tmcu \cdot XUM_{u,m}, \ \forall u, \ m \tag{S35}$$

where *tmcl* and *tmcu* are minimum and maximum capacity of pipeline transporting natural gas, respectively. $XPM_{p,m}$, $XPU_{p,u}$, and $XUM_{u,m}$ are binary variables that equal 1 if corresponding pipeline is installed between processing plant *p* and power plant *m*, processing plant *p* and underground reservoir *u*, and underground reservoir *u* and power plant *m*, respectively.

If a processing plant is established, its processing capacity should be bounded by the corresponding capacity range; otherwise, its capacity should be zero. This relationship can be modeled by the following inequality:

$$pcl \cdot YP_p \le PC_p \le pcu \cdot YP_p, \ \forall p \tag{S36}$$

where *pcl* and *pcu* are minimum and maximum capacity of processing plant, respectively.

Logic Constraints

For the drilling issue of the shale well, we have the following logic constraints.

There can be a number of wells drilled at each shale site in each time period, given by,

$$\sum_{n=0}^{mn_i} YD_{i,n,t} = 1, \ \forall i, \ t \tag{S37}$$

where $YD_{i,n,t}$ is a binary variable that equals 1 if *n* shale wells at shale site *i* are dilled in time period *t*. mn_i denotes the maximum number of wells that can be drilled at shale site *i* per time period.

The total number of wells drilled at shale site *i* in time period *t* can be calculated by,

$$NN_{i,t} = \sum_{n=0}^{mn_i} n \cdot YD_{i,n,t}, \ \forall i, \ t \tag{S38}$$

The total number of wells that can be drilled at shale site *i* over the planning horizon is bounded, given by,

$$\sum_{t \in T} NN_{i,t} \le tmn_i, \ \forall i \tag{S39}$$

where tmn_i denotes the maximum number of wells that can be drilled at shale site i over the planning horizon.

For the selection of onsite treatment technology, we note that at most one technology can be chosen. This constraint is given by,

$$\sum_{i \in I} YO_{i,o} \leq 1, \ \forall i, \ t \tag{S40}$$

Since we are conducting life cycle optimization of shale gas supply chain, with limited planning horizon, we only consider the wells that are drilled in the first several years, i.e. the first t^d time periods.

$$NN_{i,t} = 0, \ \forall i, \ t \geq t^d \tag{S41}$$

Objective Functions

Economic Objective

The economic objective is to minimize the levelized cost of electricity generated from shale gas. There are negative terms accounting for the income from sales of NGLs (I_{NGL}). Positive terms include costs related to freshwater acquisition (C_{fresh}), shale gas production operations (C_{shale}), wastewater management (C_{waste}), shale gas processing (C_{proce}), natural gas transportation (C_{TNG}), natural gas and NGL storage (C_{store}), and electricity generation (C_{power}).

I_{NGL} denotes the sales income of NGL at processing plants, which can be calculated by,

$$I_{NGL} = \sum_{p \in P} \sum_{t \in T} \frac{pl_t \cdot PLS_{p,t}}{(1+dr)^t} \tag{S42}$$

where pl_t denotes the average unit price of NGL in time period t. dr is the discount rate per time period.

C_{fresh} denotes the cost related to freshwater, including the freshwater acquisition cost and corresponding transportation cost, given by,

$$C_{fresh} = C_{freshwater}^{acquisition} + C_{freshwater}^{transport} \tag{S43}$$

The acquisition cost of freshwater is proportional to the amount of freshwater acquired from freshwater sources, calculated by,

$$C_{freshwater}^{acquisition} = \sum_{s \in S} \sum_{i \in I} \sum_{k \in K} \sum_{t \in T} \frac{fac_{s,t} \cdot FW_{s,i,k,t}}{(1+dr)^t} \tag{S44}$$

where $fac_{s,t}$ denotes the unit acquisition cost of freshwater source s in time period t.

The transportation cost with respect to freshwater includes the capital investment and variable transportation cost, given by,

$$C_{freshwater}^{transport} = \sum_{s\in S}\sum_{i\in I}\sum_{k\in K}\sum_{t\in T}\left(ftcs_{s,i,k} \cdot lfs_{s,i} \cdot XS_{s,i,k} + \frac{vtcf_k \cdot lfs_{s,i} \cdot FW_{s,i,k,t}}{(1+dr)^t} \right) \tag{S45}$$

where $ftcs_{s,i,k}$ denotes the unit capital investment of transportation mode k transporting freshwater from freshwater source s to shale site i. $lfs_{s,i}$ is the distance from freshwater source s to shale site i. $vtcf_k$ denotes the unit variable transportation cost for transportation mode k transporting freshwater.

C_{shale} indicates the cost of shale gas production operations, including the drilling cost for each well and production cost of shale gas, given by,

$$C_{shale} = \sum_{i\in I}\sum_{t\in T}\frac{sdc_{i,t} \cdot NN_{i,t}}{(1+dr)^t} + \sum_{i\in I}\sum_{t\in T}\frac{spc_{i,t} \cdot SP_{i,t}}{(1+dr)^t} \tag{S46}$$

where $sdc_{i,t}$ denotes the unit cost for shale well drilling and completion at shale site i in time period t. $spc_{i,t}$ denotes the unit cost for shale gas production at shale site i in time period t.

C_{waste} stands for the cost regarding wastewater management, which consists of the treatment and transportation cost of the chosen CWT option, underground injection and transportation cost of disposal wells, and treatment cost of onsite treatment option.

$$C_{waste} = C_{CWT}^{transport} + C_{CWT}^{treatment} + C_{disposal}^{transport} + C_{disposal}^{injection} + C_{onsite} \tag{S47}$$

Transportation costs with respect to the chosen CWT option includes the capital investment of transportation modes as well as variable costs depending on the load of transportation, given by,

$$C_{CWT}^{transport} = \sum_{i\in I}\sum_{c\in C}\sum_{k\in K}\sum_{t\in T}\left(lsc_{i,c} \cdot ftcc_{i,c,k} \cdot XC_{i,c,k} + \frac{vtcw_k \cdot lsc_{i,c} \cdot WTC_{i,c,k,t}}{(1+dr)^t} \right) \tag{S48}$$

where $lsc_{i,c}$ denotes the distance from shale site i to CWT facility c. $ftcc_{i,c,k}$ stands for the unit capital investment of transportation mode k transporting wastewater from shale site i to CWT facility c. $vtcw_k$ denotes the unit variable costs for transporting wastewater with transportation mode k.

Treatment costs regarding CWT option can be calculated by,

$$C_{CWT}^{treatment} = \sum_{i\in I}\sum_{c\in C}\sum_{k\in K}\sum_{t\in T}\frac{vc_c \cdot WTC_{i,c,k,t}}{(1+dr)^t} \tag{S49}$$

where vc_c denotes the unit costs for wastewater treatment at CWT facility c.

Transportation costs of underground disposal involves capital investment of transportation modes and corresponding operating costs, given by,

$$C_{disposal}^{transport} = \sum_{i\in I}\sum_{d\in D}\sum_{k\in K}\sum_{t\in T}\left(lsd_{i,d} \cdot ftcd_{i,d,k} \cdot XD_{i,d,k} + \frac{vtcw_k \cdot lsd_{i,d} \cdot WTD_{i,d,k,t}}{(1+dr)^t} \right) \quad \text{(S50)}$$

where $lsd_{i,d}$ denotes the distance from shale site i to disposal well d. $ftcd_{i,d,k}$ is the unit capital investment of transporting wastewater from shale site i to disposal well d using transportation mode k.

The underground injection cost of disposal wells is given by:

$$C_{disposal}^{injection} = \sum_{i\in I}\sum_{d\in D}\sum_{k\in K}\sum_{t\in T}\frac{vd_d \cdot WTD_{i,d,k,t}}{(1+dr)^t} \quad \text{(S51)}$$

where vd_d denotes the unit cost for underground injection of wastewater at disposal well d.

The cost of onsite treatment is calculated by the following equation,

$$C_{onsite} = \sum_{i\in I}\sum_{o\in O}\sum_{t\in T}\frac{vo_o \cdot WTO_{i,o,t}}{(1+dr)^t} \quad \text{(S52)}$$

where vo_o denotes the unit cost for wastewater treatment of onsite treatment technology o.

C_{proce} denotes all of the costs related to processing plants, including both the capital and operating costs for the establishment and operations of processing plants as well as the corresponding transportation activities. Note that the transportation part here indicates transporting shale gas from shale sites to processing plants. The overall relationship is expressed by,

$$C_{proce} = C_{processing}^{capital} + C_{processing}^{operating} + C_{transport}^{shalegas} \quad \text{(S53)}$$

where $C_{processing}^{capital}$ denotes the capital investment for establishing processing plants, which is proportional to the processing capacity to the power of sfp, given by,

$$C_{processing}^{capital} = \sum_{p\in P} rcp \cdot \left({PC_p}/{rpc} \right)^{sfp} \cdot \left({pci_{pp}}/{rpci_{pp}} \right) \quad \text{(S54)}$$

where rcp denotes the reference capital investment for processing plant. rpc denotes the reference capacity of processing plant. sfp denotes the size factor of processing plant. pci_{pp} denotes the chemical engineering plant cost index regarding processing plant. $rpci_{pp}$ denotes the chemical engineering plant cost index regarding processing plant of the reference year.

The total operating cost for processing plants is given by,

$$C_{processing}^{operating} = \sum_{i\in I}\sum_{p\in P}\sum_{t\in T}\frac{vp \cdot STP_{i,p,t}}{(1+dr)^t} \quad \text{(S55)}$$

where vp denotes the unit processing cost for shale gas.

We use a similar power function to calculate the capital cost of pipeline installation.[13] Thus, the transportation cost of shale gas from shale sites to processing plants is given by:

$$C_{transport}^{shalegas} = \sum_{i \in I} \sum_{p \in P} srp \cdot \left(\frac{TCP_{i,p}}{smp} \right)^{sft} \cdot \left(\frac{pci_{pl}}{rpci_{pl}} \right) \cdot lsp_{i,p} + \sum_{i \in I} \sum_{p \in P} \sum_{t \in T} \frac{vtcs \cdot lsp_{i,p} \cdot STP_{i,p,t}}{(1+dr)^t} \quad \text{(S56)}$$

where *srp* denotes the reference capital investment of pipeline transporting shale gas. *smp* denotes the reference capacity of pipeline transporting shale gas. *sft* denotes the size factor of pipeline transporting shale gas and natural gas. pci_{pp} denotes the chemical engineering plant cost index regarding gas pipeline. $rpci_{pp}$ denotes the chemical engineering plant cost index regarding pipeline of the reference year. $lsp_{i,p}$ denotes the distance from shale site *i* to processing plant *p*. *vtcs* is the unit variable transportation cost for pipeline transporting shale gas.

C_{TNG} stands for the total transportation cost of natural gas from processing plants to power plants, from processing plants to underground reservoirs, and from reservoirs to power plants, including the capital investment of pipeline construction and variable transportation cost, which can be calculated by,

$$C_{TNG} = C_{TNG}^{pm} + C_{TNG}^{pu} + C_{TNG}^{um} \quad \text{(S57)}$$

The transportation cost of natural gas directly from processing plant to power plant includes capital investment of pipeline as well as corresponding variable transportation costs, which can be calculated by,

$$C_{TNG}^{pm} = \sum_{p \in P} \sum_{m \in M} srp \cdot \left(\frac{TCPM_{p,m}}{smp} \right)^{sft} \cdot \left(\frac{pci_{pl}}{rpci_{pl}} \right) \cdot lpm_{p,m} + \sum_{p \in P} \sum_{m \in M} \sum_{t \in T} \frac{vtcm \cdot lpm_{p,m} \cdot STPM_{p,m,t}}{(1+dr)^t} \quad \text{(S58)}$$

where $lpm_{p,m}$ denotes the distance from processing plant *p* to power plant *m*. *vtcm* stands for the unit variable transportation cost for pipeline transporting natural gas.

The transportation cost of natural gas from processing plant to underground reservoir is calculated by,

$$C_{TNG}^{pu} = \sum_{p \in P} \sum_{u \in U} srp \cdot \left(\frac{TCPU_{p,u}}{smp} \right)^{sft} \cdot \left(\frac{pci_{pl}}{rpci_{pl}} \right) \cdot lpu_{p,u} + \sum_{p \in P} \sum_{u \in U} \sum_{t \in T} \frac{vtcm \cdot lpu_{p,u} \cdot STPU_{p,u,t}}{(1+dr)^t} \quad \text{(S59)}$$

where $lpu_{p,u}$ denotes the distance from processing plant *p* to underground reservoir *u*.

The transportation cost of natural gas from underground reservoir to power plant is given by,

$$C_{TNG}^{um} = \sum_{u \in U} \sum_{m \in M} srp \cdot \left(\frac{TCUM_{u,m}}{smp} \right)^{sft} \cdot \left(\frac{pci_{pl}}{rpci_{pl}} \right) \cdot lum_{u,m} + \sum_{u \in U} \sum_{m \in M} \sum_{t \in T} \frac{vtcm \cdot lum_{u,m} \cdot STUM_{u,m,t}}{(1+dr)^t} \quad \text{(S60)}$$

where $lum_{u,m}$ denotes the distance from underground reservoir *u* to power plant *m*.

C_{store} denotes the total cost of underground natural gas storage as well as NGL storage, which is proportional to their storage amount, given by,

$$C_{store} = \sum_{u\in U}\sum_{t\in T}\frac{\sum_{p\in P} vui_u \cdot STPU_{p,u,t} + \sum_{m\in M} vuw_u \cdot STUM_{u,m,t}}{\left(1+dr\right)^t} + \sum_{p\in P}\sum_{t\in T}\frac{vs \cdot SPS_{p,t}}{\left(1+dr\right)^t} \quad \text{(S61)}$$

where vui_u denotes the unit injection cost at underground reservoir u. vuw_u denotes the unit withdrawal cost at underground reservoir u. vs denotes the storage cost of NGL at processing plant.

C_{power} denotes the operating cost proportional to the amount of natural gas for electricity generation, calculated by,

$$C_{power} = \sum_{m\in M}\sum_{t\in T}\frac{ve_m \cdot \left(\sum_{p\in P} STPM_{p,m,t} + \sum_{u\in U} STUM_{u,m,t}\right)}{\left(1+dr\right)^t} \quad \text{(S62)}$$

where ve_m denotes the unit cost for electricity generation from natural gas at power plant m.

The levelized cost of electricity is a long-term cost concept, which represents a “breakeven” value that a power provider would need to charge in order to justify the investment in a particular energy project. The levelized cost of electricity is expressed as the total life cycle cost, which is denoted as TC, divided by the total lifetime electricity generation, denoted as TGE, given by,

$$\min\ LC = \frac{TC}{TGE} = \frac{C_{freshwater} + C_{shale} + C_{wastewater} + C_{processing} + C_{TNG} + C_{storage} + C_{power} - I_{NGL}}{\sum_{m\in M}\sum_{t\in T} GE_{m,t}} \quad \text{(S63)}$$

Environmental Objective

The environmental objective is to minimize the GHG footprint associated with generation of unit electricity by natural gas from the shale gas production network (UE), accounting for GHG emissions from freshwater acquisition (E_{fresh}), shale well drilling, stimulation, and completion (E_{drill}), shale gas production (E_{produ}), wastewater management (E_{waste}), shale gas transportation (E_{TSG}), shale gas processing (E_{proce}), natural gas transportation (E_{TNG}), natural gas and NGL storage (E_{store}), and electricity generation (E_{power}). The 100-year global warming potential is employed here to quantify the life cycle impact assessment of GHG emissions.[13,20,21]

The emissions corresponding to freshwater acquisition is mainly due to the use of liquid transportation fuels for trucks or electricity input for pumping in the pipeline transportation mode, which is proportional to the amount of freshwater being transported. [8]

$$E_{fresh} = \sum_{s\in S}\sum_{i\in I}\sum_{k\in K}\sum_{t\in T} eft_k \cdot lfs_{s,i} \cdot FW_{s,i,k,t} \quad \text{(S64)}$$

where eft_k denotes emissions associated with transportation of unit amount of freshwater by transportation mode k.

The emissions during shale well drilling process is the total emissions before the shale well is ready for shale gas production; a series of processes including well pad construction, drilling, stimulation, and completion are considered.[8]

$$E_{drill} = \sum_{i\in I}\sum_{t\in T} esd_i \cdot NN_{i,t} \tag{S65}$$

where esd_i denotes the emissions associated with the drilling process of a shale well at shale site i.

The emissions during the shale gas production process mainly stems from fracturing fluid additive manufacture, sand mining, energy usage of pump and compressors, hydraulic fracturing, workover flowback, venting, field separation, and corresponding transportation, etc.[5]

$$E_{produ} = \sum_{i\in I}\sum_{t\in T} ewf_i \cdot SP_{i,t} \tag{S66}$$

where ewf_i denotes the emissions associated with the production process of unit shale gas at shale site i.

The emissions from water management includes emissions from wastewater injection into disposal wells, from CWT facilities, onsite treatment facilities as well as corresponding transportation processes.[8, 19]

$$E_{waste} = E_{wastewater}^{CWT} + E_{wastewater}^{disposal} + E_{wastewater}^{onsite} \tag{S67}$$

The emissions corresponds to CWT option is calculated by,

$$E_{wastewater}^{CWT} = \sum_{i\in I}\sum_{c\in C}\sum_{k\in K}\sum_{t\in T} ewt_k \cdot lsc_{i,c} \cdot WTC_{i,c,k,t} + \sum_{i\in I}\sum_{c\in C}\sum_{k\in K}\sum_{t\in T} ewc_c \cdot WTC_{i,c,k,t} \tag{S68}$$

where ewt_k denotes the emissions associated with transportation of unit amount of wastewater by transportation mode k. ewc_c denotes the emissions associated with treatment of unit amount of wastewater at CWT facility c.

The emissions from wastewater being injected into disposal wells is calculated by,

$$E_{wastewater}^{disposal} = \sum_{i\in I}\sum_{d\in D}\sum_{k\in K}\sum_{t\in T} ewt_k \cdot lsd_{i,d} \cdot WTD_{i,d,k,t} + \sum_{i\in I}\sum_{d\in D}\sum_{k\in K}\sum_{t\in T} ewd_d \cdot WTD_{i,d,k,t} \tag{S69}$$

where ewd_d denotes the emissions associated with underground injection of unit amount of wastewater at disposal well d.

The emissions for onsite wastewater treatment is given by,

$$E_{wastewater}^{onsite} = \sum_{i\in I}\sum_{o\in O}\sum_{t\in T} ewo_o \cdot WTO_{i,o,t} \tag{S70}$$

where ewo_o denotes the emissions associated with treatment of unit amount of wastewater by onsite treatment technology o.

The emissions for the shale gas transportation is largely due to the energy input for pipeline transportation as well as leakage during long distance transmission, which is proportional to both the transportation load and distance.[20]

$$E_{TSG} = \sum_{i \in I} \sum_{p \in P} \sum_{t \in T} est \cdot lsp_{i,p} \cdot STP_{i,p,t} \tag{S71}$$

where *est* denotes the emissions associated with transportation of unit amount of shale gas by pipeline.

The emissions from shale gas processing mainly derive from energy consumption in the processing plant and processing fugitive emissions, which are dependent on the processing amount of shale gas.

$$E_{proce} = \sum_{i \in I} \sum_{p \in P} \sum_{t \in T} esp_p \cdot STP_{i,p,t} \tag{S72}$$

where esp_p denotes the emissions associated with processing process of unit amount of shale gas at processing plant *p*.

The emissions regarding natural gas transportation is related to the energy consumption and fugitive emissions during the pipeline transportation processes, including transportation from processing plant to power plant, from processing plant to underground reservoir, and from underground reservoir to power plant. These emissions depends on the distance and amount of natural gas being transported.[7]

$$E_{TNG} = E_{TNG}^{pm} + E_{TNG}^{pu} + E_{TNG}^{um} \tag{S73}$$

The emissions of transporting natural gas from processing plant to power plant is calculated by,

$$E_{TNG}^{pm} = \sum_{p \in P} \sum_{m \in M} \sum_{t \in T} emt \cdot lpm_{p,m} \cdot STPM_{p,m,t} \tag{S74}$$

where *emt* denotes the emissions associated with transportation of unit amount of natural gas by pipeline.

The emissions of transporting natural gas from processing plant to underground reservoir is given by,

$$E_{TNG}^{pu} = \sum_{p \in P} \sum_{u \in U} \sum_{t \in T} emt \cdot lpu_{p,u} \cdot STPU_{p,u,t} \tag{S75}$$

The emissions of transporting natural gas from underground reservoir to power plant is calculated by,

$$E_{TNG}^{um} = \sum_{u \in U} \sum_{m \in M} \sum_{t \in T} emt \cdot lum_{u,m} \cdot STUM_{u,m,t} \tag{S76}$$

The emissions from storage includes the storage of NGL as well as underground storage of natural gas, which is related to the energy consumption of injection, withdrawal, and compression operations as well as fugitive emissions during inventory and these processes.[5, 21]

$$E_{store} = E_{storage}^{NGL} + E_{storage}^{NG} \tag{S77}$$

The emissions during storage of NGL is dependent on the inventory level and storage time of NGL, given by,

$$E_{storage}^{NGL} = \sum_{p \in P} \sum_{t \in T} els_{p,t} \cdot SPS_{p,t} \tag{S78}$$

where $els_{p,t}$ denotes the emissions associated with storage of unit amount of NGL at processing plant p in time period t.

The emissions from the underground storage of natural gas is related not only to the inventory level, but also to the injection and withdrawal load in each time period, calculated by,

$$E_{storage}^{NG} = \sum_{p \in P} \sum_{u \in U} \sum_{t \in T} emi_{u,t} \cdot STPU_{p,u,t} + \sum_{u \in U} \sum_{t \in T} ems_{u,t} \cdot URS_{u,t} + \sum_{u \in U} \sum_{m \in M} \sum_{t \in T} emw_{u,t} \cdot STUM_{u,m,t} \tag{S79}$$

where $emi_{u,t}$ denotes the emissions associated with injection of unit amount of natural gas at underground reservoir u at time period t. $ems_{u,t}$ denotes the emissions associated with underground storage of unit amount of natural gas at underground reservoir u in time period t. $emw_{u,t}$ is the emissions associated with withdrawal of unit amount of natural gas at underground reservoir u in time period t

The emissions during electricity generation depends on the combustion load, converting efficiency, fugitive emissions, etc. This emissions is proportional to the amount of electricity generated at the power plant.

$$E_{power} = \sum_{m \in M} \sum_{t \in T} emp_{m,t} \cdot GE_{m,t} \tag{S80}$$

where $emp_{m,t}$ denotes the emissions associated with electricity generation from a unit amount of natural gas at power plant m in time period t

The life cycle boundary in this model is specified as “well-to-wire”, where the transmission and end use of electricity are not considered. The life cycle stages include freshwater acquisition, shale well construction, shale gas production, wastewater management, transportation, shale gas processing, and inventory. The environmental objective is defined as the total environmental impact of shale gas throughout the shale gas supply chain, which is denoted as TE, divided by the total amount of electricity generated. As discussed in the Section 2.2, we apply a functional-unit-based LCA optimization framework; therefore, a fractional objective function is employed here to evaluate the environmental impacts.[5]

$$UE = \frac{TE}{TGE} = \frac{\left(E_{fresh} + E_{drill} + E_{produ} + E_{waste} + E_{TSG} + E_{proce} + E_{TNG} + E_{store} + E_{power}\right)}{\sum_{m \in M} \sum_{t \in T} GE_{m,t}} \tag{S81}$$

Tailored Global Optimization Algorithm

The ε-constraint method is widely used to obtain Pareto-optimal solutions for multiobjective optimization problems, mainly because of its efficiency and simplicity. Based on this method, the environmental objective can be converted into an ε-constraint while leaving only the economic objective in the resulting single-objective ε-constraint subproblem. The resulting problem is one kind of mixed-integer fractional programming (MIFP) problem. Due to non-convexity and the presence of integer variables, solving large-scale MIFP problems directly using general-purpose MINLP methods can be computationally intractable. The parametric algorithm is known as an efficient tailored algorithm for solving MIFP problems.[22-24] The basic idea is to transform the original MIFP problem into a set of parametric subproblems, such that the fractional form is removed, and less nonlinearity is obtained, making the resulting MINLP problem easier to solve. According to this solution method, we consider the following parametric problem,

$$\min \quad F(LC) = TC - LC \cdot TGE$$

$$\text{s.t.} \quad TE \le \varepsilon \cdot TGE \quad \varepsilon\text{-constraint}$$

(P1)

Mass Balance Constraints (S1)-(S12)
Capacity Constraints (S13)-(S26)
Composition Constraints (S27)
Bounding Constraints (S28)-(S36)
Logic Constraints (S37)-(S41)
Economic Constraints (S42)-(S62)
Environmental Constraints (S64)-(S80)

As can be seen, the new objective function *F(LC)* is actually a function of parameter *LC*, which is also the original objective value that we try to obtain. One important property of this function *F(LC)* is that both problem (P0) and (P1) share the same global optimal solution if we find a parameter LC^* such that $F(LC^*) = 0$. Therefore, to solve problem (P1), the major task is to find the root of the equation $F(LC) = 0$. In principle, various root-finding methods can be employed to solve this parametric problem.[22, 25] In this work, the parametric algorithm based on an in-exact Newton's method is applied to tackle this MIFP problem. The detailed procedure of this algorithm is as follows,

Step 1. Set $LC = 0$ in the first iteration, and set $n = 1$;

Step 2. Solve problem (P1) with 10% relative optimality gap, and denote the solution as TC^* and TGE^*.

Step 3. If $F(LC) < \delta$, stop and output *LC* as the optimal objective value; otherwise, update $LC = TC^* / TGE^*$, set $n = n + 1$, and go to step 2.

Due to the concave terms regarding capital cost in the objective function, in each iteration of Step 2, an MINLP problem (P1) is solved. In order to further improve the computational efficiency, a branch-and-refine algorithm based on successive piecewise linear approximations is introduced to tackle the remaining concave terms in the parametric objective function.[3, 26-28]

One typical concave term is the power function (S54) with the exponent of *sfp*,

$$C_{processing}^{capital} = \sum_{p \in P} cc_p^{pc} = \sum_{p \in P} rcp \cdot \left(PC_p / rpc \right)^{sfp} \cdot \left(pci_{pp} / rpci_{pp} \right)$$

where cc_p^{pc} denotes the capital cost regarding processing plant *p*.

In this work, the piecewise linear approximation is derived using specially ordered set variables of type 2 (SOS2).[29] Thus, the above concave term is approximated with the following equations,

$$cc_p^{pc} = \sum_{pt \in PT} pcc_{p,pt}^{pc} \cdot y_{p,pt}^{pc}, \ \forall p \tag{82}$$

$$PC_p = \sum_{pt \in PT} pcap_{p,pt}^{pc} \cdot y_{p,pt}^{pc}, \ \forall p \tag{83}$$

$$\sum_{pt \in PT} y_{p,pt}^{pc} = 1, \ \forall p \tag{84}$$

$$y_{p,pt}^{pc} \in \{\text{SOS2 variables}\} \tag{85}$$

where the set of grid points is indexed by *pt*. $pcap_{p,pt}^{pc}$ is the capacity of processing plant corresponding to pre-specified grid points. $pcc_{p,pt}^{pc}$ stands for the capital cost of processing plant corresponding to pre-specified grid points. $y_{p,pt}^{pc}$ is defined as SOS2 variables, which have the following properties: at most two variables within a SOS2 can take on non-zero values. The two non-zero values have to be for adjacent variables in that set.

Based on the SOS2 formulation (1)-(4), the concave terms in (S54), (S56), (S58)-(S60) for calculating the capital costs can be approximated by the piecewise linear approximations. Therefore, the original MINLP subproblem is approximated by an MILP subproblem. Here (P2) denotes this MILP problem based on piecewise linear approximations.

(P2)

$$\min \quad F(LC) = TC^{approx} - LC \cdot TGE$$

s.t. $TE \le \varepsilon \cdot TGE$ ε-constraint

Mass Balance Constraints (S1)-(S12)

Capacity Constraints (S13)-(S26)

Composition Constraints (S27)

Bounding Constraints (S28)-(S36)

Logic Constraints (S37)-(S41)

Economic Constraints (S42)-(S62)

Environmental Constraints (S64)-(S80)

By solving this MILP problem (P2), a lower bound for the objective value of original MINLP problem (P1) can be obtained. Meanwhile, since the optimal solution of (P2) is always a feasible solution for the MINLP problem (P2), by substituting the optimal solution of MILP problem into the MINLP problem, an upper bound for the objective function of (P1) is obtained.

Next, the improved branch-and-refine algorithm is presented to provide a global optimization of the MINLP problem.[30-31] The branch-and-refine algorithm include the following procedures,

***Step 1*. Initialization**

Set iteration count $iter = 0$, lower bound $LB = -\infty$, upper bound $UB = +\infty$. Specify the initial partitioning point and construct the piecewise linear approximation.

***Step 2*. Solve MILP subproblem**

Set $iter = iter + 1$. Solve the MILP subproblem (P2), if feasible, denote the optimal objective value as obj^{LB} and update $LB = \max(obj^{LB}, LB)$; substitute the optimal solution into original nonlinear objective function, denote the objective value as obj^{UB}, and update $UB = \min(obj^{UB}, UB)$.

***Step 3*. Check convergence**

If $\left|(UB - LB)/LB\right| < tol$, stop and output the current solution as the optimal solution; otherwise, go to the next step.

***Step 4*. Grid propagation**

Add a grid point right at the optimal value to improve the approximation, update all the parameters involved, and go to step 2.

By integrating the branch-and-refine algorithm and the parametric algorithm, it is possible to transform the global optimization of original MIFP problem into solving a sequence of MILP subproblems. The full procedure of this algorithm is summarized in Figure S3.

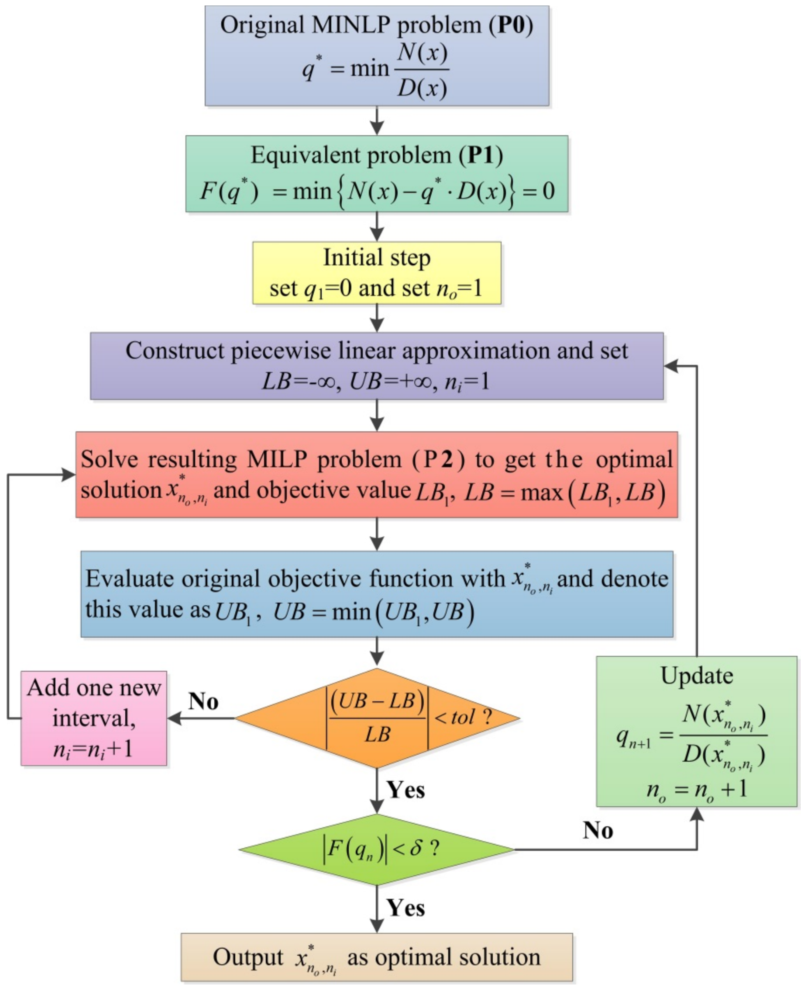

Figure S3. Flowchart of branch-and-refine Integrated parametric algorithm

Small Scale Case Study

In this section, we present the small case study verifying the proposed algorithm.

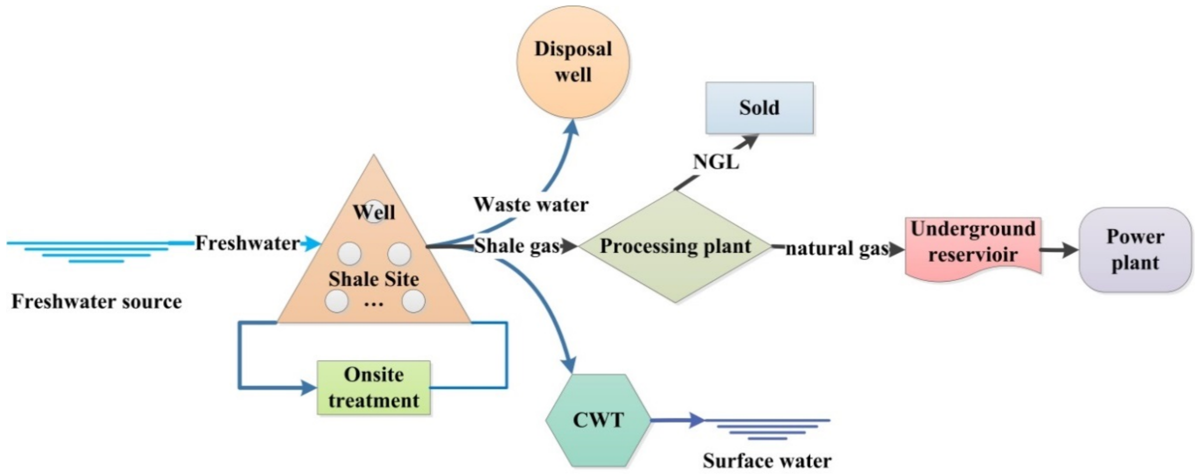

Figure S4. Superstructure of the shale gas supply chain in small case

In this small case study, we only consider 1 freshwater source, 1 shale site with maximum 4 potential wells to drill, 1 disposal well, 1 CWT facility, 3 onsite treatment technologies, 1 processing plant, 1 underground reservoir as depleted natural gas field, and 1 power plant. The planning horizon is 2 years, divided into 8 quarters. Wells are assumed to be drilled in the first two quarters. A detailed superstructure of this supply chain is given in Figure S4.

Since the main objective is to verify the proposed algorithm, we only consider the economic objective here. We apply the proposed global optimization algorithm to solve the resulting problem. In addition, we use general-purpose global optimizers BARON 14 as well as SCIP 3 to solve this problem. The corresponding model statistics and computational results are summarized in Table S1. As can be seen, all three solution methods obtain the same optimal solution, which verifies the feasibility and efficiency of the proposed branch-and-refine integrated parametric algorithm.

Table S1. Model and Solution Statistics of the Proposed Solution Methods

Method	BARON 14	SCIP 3	B&R + Parametric
# of discrete variables	19	19	19
# of continuous variables	121	121	146
# of constraints	186	186	195
Number of iterations	1	1	3 (outer loop) 7 (inner loop)
Objective ($/MWh)	439	439	439
Total CPU time (s)	15.3	3,600[a]	0.3

a. Failed to converge to global optimality within 3,600 CPU seconds

Computational Performance

The Pareto-optimal curve in Figure 3 is composed of 10 optimal points, and the total computational time is 122.5 hours. To demonstrate the performance of the proposed branch-and-refine integrated parametric algorithm, we consider point B for illustration.

We note that though the scale of this problem is not extremely large, due to the combinatorial nature and non-convex property of the MIFP problem, off-the-shelf global optimizers, namely BARON 14 and SCIP 3, failed to return any feasible solution even after running for a week. In this section, we present the resulting upper and lower bounds of each iteration of the optimization problem of point B, which is shown in Table S2. The integrated algorithm takes four outer iterations to find the optimal objective value of problem (P2), and for each outer iteration, it takes two to five inner iterations to converge. We note that during the inner loop, the upper bound decreases while the lower bounds increases until they are close enough to satisfy the inner stopping criterion. We can observe a significant improvement in each iteration, and in the last one, both lower bound and upper bound converge to 0.

Table S2. Lower and upper bounds in solving the optimization problem of point B

Outer iteration	Parameter *LC*	Inner iteration	Lower bound	Upper bound
1	60	1	1,183,330.838	1,214,570.481
	60	2	1,210,602.449	1,214,570.481
2	71	1	-427,878.622	-386,933.532
	71	2	-392,988.771	-386,933.532
	71	3	-392,988.771	-392,561.809
3	69	1	-38,768.875	1,999.976
	69	2	-5,527.717	1,999.976
	69	3	1,491.652	1,591.976
	69	4	1,542.378	1,542.378
4	69	1	-37,934.853	6,023.513
	69	2	-4,502.799	6,023.513
	69	3	-1,423.933	0
	69	4	-0.007	0
	69	5	0	0

Sensitivity Analysis

In this section, we present a sensitivity analysis regarding the shale well lifetime. As can be seen in Figure S5, we consider different shale well lifetime assumptions, including 6 years, 8 years, 10 years, 12 years, 15 years, 18 years, and 20 years. The rest of input data are kept identical. By solving the corresponding optimization problems, we obtain a series of LCOEs. In general, the LCOE is not sensitive to the lifetime assumption. From 6 years to 12 years, the same LCOE is obtained. However, when the shale well lifetime is longer than 15 years, the corresponding LCOE is slightly higher. The highest LCOE is observed with 20-year lifetime, resulting in only a 5% discrepancy. Such a result is consistent with our knowledge regarding the average Marcellus shale play lifetime.[10] Based on this analysis, we come to the conclusion that the assumption on shale well lifetime, though leading to minor differences in economic performances of this model, will not result in any significant change. In addition, it is worth noting that the estimated ultimate recovery (EUR) of shale well is identified as an important factor in recent studies, the uncertainties of which can lead to significant discrepancy in the overall shale gas performance. We will address this problem in future work using an advanced stochastic programming approach.

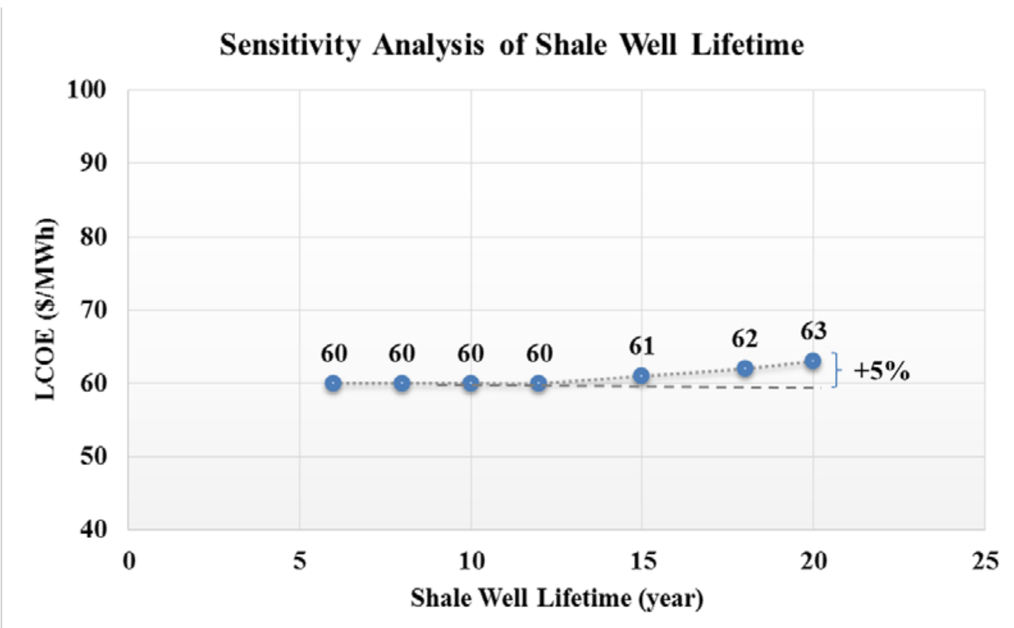

Figure S5. Sensitivity analysis of shale well lifetime

Input Data for the Case Studies

The estimated shale gas production profile of shale well is depicted in Figure S6.

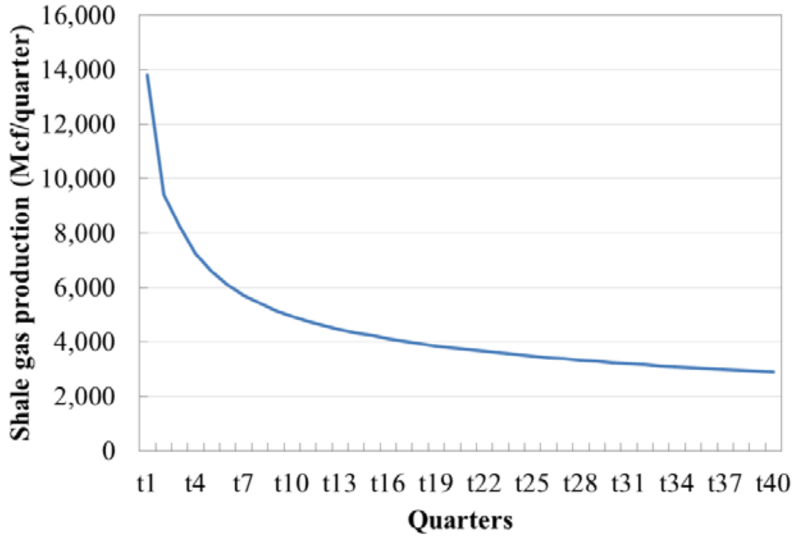

Figure S6. Estimation of shale gas production profile[13]

The parameters employed in this model are listed in the following tables.

Table S3. Economic parameters

Parameters	Values/Reference	Descriptions
$cc_{i,\tau}$ (bbl/mcf)	0.05-0.01/[8]	Correlation coefficient for shale gas production and wastewater production of a shale well at shale site *i*
$cca_{c,t}$ (bbl/quarter)	150,000-600,000/[32]	Capacity for wastewater treatment at CWT facility *c* in time period *t*
$dca_{d,t}$ (bbl/quarter)	15,000-90,000/[32]	Capacity for underground injection at disposal well *d* in time period *t*
dl_t (mcf/quarter)	1,200-1,800/[13]	Minimum demand for NGL in time period *t*
$dlup_t$ (mcf/quarter)	120,000-180,000/[13]	Maximum demand for NGL in time period *t*
$dm_{m,t}$ (mcf/quarter)	4,800-7,200/[13]	Minimum demand of natural gas at power plant *m* in time period *t*
$dmup_{m,t}$ (mcf/quarter)	480,000-720,000/[13]	Maximum demand of natural gas at power plant *m* in time period *t*
dr (quarterly)	0.024/[13]	Discount rate per time period
$fac_{s,t}$ ($/bbl)	0.04-0.06/[15]	Unit acquisition cost of freshwater at freshwater source s in time period *t*
$fca_{s,t}$ (bbl/quarter)	150,000-6,000,000/[33]	Available freshwater supply capacity at freshwater source *s* in time period *t*
$ftcc_{i,c,k}$ ($/mile)	*k1*: 800; *k2*: 3,500/[15, 18]	Unit capital investment of transportation mode *k* transporting wastewater from shale site *i* to CWT facility *c*
$ftcd_{i,d,k}$ ($/mile)	*k1*: 800; *k2*: 3,500/[15, 18]	Unit capital investment of transportation mode *k* transporting wastewater from shale site *i* to disposal well *d*
$ftcs_{s,i,k}$ ($/mile)	*k1*: 800; *k2*: 3,000/[15, 18]	Unit capital investment of transportation mode *k* transporting freshwater from freshwater source *s* to shale site *i*
lc_i	0.1-0.2/[13]	NGL composition in shale gas at shale site *i*
$lfs_{s,i}$ (mile)	5-30/[15]	Distance from freshwater source *s* to shale site *i*
lo_o	*o1*: 0.15; *o2*: 0.45; *o3*: 0.65/[18]	Recovery factor for treating wastewater of onsite treatment technology *o*

$lpm_{p,m}$ (mile)	5-60/[13]	Distance from processing plant *p* to power plant *m*
$lpu_{p,u}$ (mile)	5-20/[13]	Distance from processing plant *p* to underground reservoir *u*
$lsc_{i,c}$ (mile)	10-30/[15]	Distance from shale site *i* to CWT facility *c*
$lsd_{i,d}$ (mile)	50-150/[15]	Distance from shale site *i* to disposal well *d*
$lsp_{i,p}$ (mile)	5-30/[13]	Distance from shale site *i* to processing plant *p*
$lum_{p,m}$ (mile)	5-20/[13]	Distance from underground reservoir *u* to power plant *m*
mc_i	0.8-0.9/[13]	Methane composition in shale gas at shale site *i*
mn_i	2/[13]	Maximum number of wells that can be drilled at shale site *i* per time period
ocl_o (bbl/quarter)	*o1*: 30; *o2*: 20; *o3*: 15/[32]	Minimum treatment capacity for onsite treatment technology *o*
ocu_o (bbl/quarter)	*o1*: 60,000; *o2*: 10,000; *o3*: 6,000/[32]	Maximum treatment capacity for onsite treatment technology *o*
pci_{pl}	881.9/[34]	Chemical engineering plant cost index for pipeline
pci_{pp}	574/[34]	Chemical engineering plant cost index for processing plant
pcl (mcf/quarter)	30,000/[13]	Minimum capacity of processing plant
pcu (mcf/quarter)	5,000,000/[13]	Maximum capacity of processing plant
pef	0.97/[13]	Processing efficiency of shale gas
pl_t ($/mcf gas)	10-15/[35]	Average unit price of NGL in time period *t*
psc_p (mcf/quarter)	90,000/[13]	Minimum storage capacity of NGL for each time period at processing plant *p*
rcp ($)	21,310,000/[14]	Reference capital investment for processing plant
rf_o	*o1*: 0.43; *o2*: 0.40; *o3*: 0.38/[18]	Ratio of freshwater to wastewater required for blending after treatment of onsite treatment technology *o*

rpc (mcf/quarter)	4,809,600/[14]	Reference capacity of processing plant
$rpci_{pl}$	887.6/[34]	Chemical engineering plant cost index of the reference year for pipeline
$rpci_{pp}$	567.3/[34]	Chemical engineering plant cost index of the reference year for processing plant
$sdc_{i,t}$ ($)	270,000-292,000/[8]	Unit cost for shale well drilling and completion at shale site i in time period t
sfp	0.6/[13]	Size factor of processing plant
sft	0.6/[13]	Size factor of pipeline transporting shale gas and natural gas
smm (mcf/quarter)	639,840/[13]	Reference capacity of pipeline transporting natural gas
smp (mcf/quarter)	639,840/[13]	Reference capacity of pipeline transporting shale gas
$spc_{i,t}$ ($/mcf)	0.4-0.6/[8]	Unit cost for shale gas production at shale site i in time period t
$spp_{i,\tau}$ (mcf/quarter)	$spp_{i,\tau} = a \cdot t^{b}$; a:16,000-18,000; b:-0.37/[13]	Shale gas production of a shale well of age τ at shale site i
srm ($/mile)	64,144/[13]	Reference capital investment of pipeline transporting natural gas
srp ($/mile)	64,144/[13]	Reference capital investment of pipeline transporting shale gas
$tcc_{i,c,k}$ (bbl/quarter)	$k1$: 135,000; $k2$: 1,200,000/[15, 18]	Transportation capacity for transportation mode k from site i to CWT facility c
$tdc_{i,d,k}$ (bbl/quarter)	$k1$: 135,000; $k2$: 1,200,000/[15, 18]	Transportation capacity for transportation mode k from site i to disposal well d
$tmcl$ (mcf/quarter)	9,000/[13]	Minimum capacity of pipeline transporting natural gas
$tmcu$ (mcf/quarter)	210,000,000/[13]	Maximum capacity of pipeline transporting natural gas
tmn_i	4-8/[36]	Maximum number of wells that can be drilled at shale site i over planning horizon
$tpcl$ (mcf/quarter)	9,000/[13]	Minimum capacity of pipeline transporting shale gas
$tpcu$ (mcf/quarter)	210,000,000/[13]	Maximum capacity of pipeline transporting shale gas
$tsc_{s,i,k}$ (bbl/quarter)	$k1$: 135,000; $k2$: 1,200,000/[15, 18]	Transportation capacity for transportation mode k from source s to shale site i
uca_u (mcf/quarter)	32,400,000/[21]	Working gas capacity of underground reservoir u

ue (kWh/mcf)	135.7/[4]	Amount of electricity generated per unit natural gas input
uic_u (mcf/quarter)	9,000,000/[21]	Injection capability for each time period of underground reservoir u
uwc_u (mcf/quarter)	18,240,000/[21]	Withdrawal capability for each time period of underground reservoir u
vc_c (\$/bbl)	3.2-3.8/[18]	Unit cost for wastewater treatment at CWT facility c
vd_d (\$/bbl)	1.0-1.4/[18]	Unit cost for underground injection of wastewater at disposal well d
ve_m (\$/mcf)	1.45-1.49/[37]	Unit cost for electricity generation from natural gas at power plant m
vo_o (\$/bbl)	$o1$: 6.5; $o2$: 5.4; $o3$: 4.7/[38]	Unit cost for wastewater treatment of onsite treatment technology o
vp (\$/mcf)	6.3/[14]	Unit processing cost for shale gas
vs (\$/mcf)	0.1/[35]	Unit storage cost for NGL
$vtcf_k$ (\$/(bbl·mile))	$k1$: 0.02; $k2$: 0.0004/[15, 18]	Unit variable transportation cost for transportation mode k transporting freshwater
$vtcm$ (\$/(mcf·mile))	0.0015/[13]	Unit variable transportation cost for pipeline transporting natural gas
$vtcs$ (\$/(mcf·mile))	0.0015/[13]	Unit variable transportation cost for pipeline transporting shale gas
$vtcw_k$ (\$/(bbl·mile))	$k1$: 0.03; $k2$: 0.0006/[15, 18]	Unit variable transportation cost for transportation mode k transporting wastewater
vui_u (\$/mcf)	0.02/[39]	Unit injection cost at underground reservoir u
vuw_u (\$/mcf)	0.01/[39]	Unit withdrawal cost at underground reservoir u
wd_i (bbl/well)	2,500-3,200/[8]	Average drilling water usage for each well at shale site i
wrd_i	0.10-0.15/[18]	Recovery ratio of water for drilling process at shale site i
wrf_i	0.15-0.25/[18]	Recovery ratio of water for hydraulic fracturing process at shale site i

Table S4. Environmental parameters

Parameters	Values	Descriptions
eft_k (g CO_2e/(bbl·mile))	*k1*: 1.31;*k2*: 0.44/[8]	Emissions associated with transporting unit freshwater by transportation mode *k*
esd_i (g CO_2e/well)	281,000-321,000/[5]	Emissions associated with the drilling process of a shale well at shale site *i*
ewf_i (g CO_2e/mcf)	3,500-5,990/[4, 40]	Emissions associated with the production process of unit shale gas at shale site *i*
ewt_k (g CO_2e/(bbl·mile))	*k1*: 1.31; *k2*: 0.44/[8]	Emissions associated with transporting unit wastewater by transportation mode *k*
est (g CO_2e/(mcf·mile))	57/[4]	Emissions associated with transportation of unit amount of shale gas by pipeline
ewd_d (g CO_2e/bbl)	1,000-1,040/[41]	Emissions associated with injecting unit wastewater at disposal well *d*
ewc_c (g CO_2e/bbl)	1,260-1,300/[42]	Emissions associated with treating unit wastewater at CWT facility *c*
ewo_o (g CO_2e/bbl)	*o1*: 3,797; *o2*: 2,813; *o3*: 350/[19, 38]	Emissions associated with treating unit wastewater by onsite treatment technology *o*
esp_p (g CO_2e/mcf)	4,253-5,453/[4]	Emissions associated with processing process of unit amount of shale gas at processing plant *p*
$els_{p,t}$ (g COe/mcf gas)	780-840/[4]	Emissions associated with storage of unit amount of NGL at processing plant *p* in time period *t*
emt (g CO_2e/(mcf·mile))	57/[4, 40]	Emissions associated with transportation of unit amount of natural gas by pipeline
$ems_{u,t}$ (g CO_2e/mcf)	287-337/[20-21]	Emissions associated with underground storage of unit amount of natural gas at underground reservoir *u* in time period *t*
$emi_{u,t}$ (g CO_2e/mcf)	1,171-1,571/[20-21]	Emissions associated with injection of unit amount of natural gas at underground reservoir *u* in time period *t*
$emw_{u,t}$ (g CO_2e/mcf)	603-663/[20-21]	Emissions associated with withdrawal of unit amount of natural gas at underground reservoir *u* in time period *t*
$emp_{m,t}$ (g CO_2e/kWh)	303-423/[5, 40]	Emissions associated with electricity generation of unit amount of natural gas at power plant *m* in time period *t*

Nomenclature

Sets

C	Set of CWT treatment facilities indexed by *c*
D	Set of different disposal wells indexed by *d*
I	Set of shale sites indexed by *i*
K	Set of transportation modes indexed by *k* (*k1*: truck; *k2*: pipeline)
M	Set of power plants indexed by *m*
N	Set of number of wells indexed by *n*
O	Set of onsite treatment technologies indexed by *o* (*o1:* MSF; *o2*: MED; *o3*: RO)
P	Set of processing plants indexed by *p*
S	Set of freshwater resources indexed by *s*
T	Set of time periods indexed by *t*
U	Set of underground reservoirs indexed by *u*

Subset

$T'(t)$	Subset of time periods when wells are drilled indexed by *t'*

Subscripts/Superscripts

pp	Processing plant
pl	Pipeline

Parameters

cc_i	Correlation coefficient for shale gas production and wastewater production of a shale well at shale site *i*
$cca_{c,t}$	Capacity for wastewater treatment at CWT facility c in time period t
$dca_{d,t}$	Capacity for underground injection at disposal well d in time period t
dl_t	Minimum demand for NGL in time period *t*

$dlup_t$	Maximum demand for NGL in time period *t*
$dm_{m,t}$	Minimum demand of natural gas at power plant *m* in time period t
$dmup_{m,t}$	Maximum demand of natural gas at power plant *m* in time period t
dr	Discount rate per time period
eft_k	Emissions associated with transportation of unit amount of freshwater by transportation mode *k*
$els_{p,t}$	Emissions associated with storage of unit amount of NGL at processing plant *p* in time period *t*
$emi_{u,t}$	Emissions associated with injection of unit amount of natural gas at underground reservoir *u* in time period *t*
$emp_{m,t}$	Emissions associated with electricity generation of unit amount of natural gas at power plant *m* in time period *t*
$ems_{u,t}$	Emissions associated with underground storage of unit amount of natural gas at underground reservoir *u* in time period *t*
emt	Emissions associated with transportation of unit amount of natural gas by pipeline
$emw_{u,t}$	Emissions associated with withdrawal of unit amount of natural gas at underground reservoir *u* in time period *t*
esd_i	Emissions associated with the drilling process of a shale well at shale site *i*
esp_p	Emissions associated with processing process of unit amount of shale gas at processing plant *p*
est	Emissions associated with transportation of unit amount of shale gas by pipeline
ewc_c	Emissions associated with treatment of unit wastewater at CWT facility *c*
ewd_d	Emissions associated with underground injection of unit wastewater at disposal well *d*
ewf_i	Emissions associated with the production process of unit shale gas at shale site *i*
ewo_o	Emissions associated with treating unit wastewater by onsite treatment technology *o*
ewt_k	Emissions associated with transportation of unit wastewater by transportation mode *k*
$fac_{s,t}$	Unit acquisition cost of freshwater at freshwater source *s* in time period *t*
$fca_{s,t}$	Available freshwater supply capacity at freshwater source *s* in time period *t*

$ftcc_{i,c,k}$	Unit capital investment of transportation mode k transporting wastewater from shale site i to CWT facility c
$ftcd_{i,d,k}$	Unit capital investment of transportation mode k transporting wastewater from shale site i to disposal well d
$ftcs_{s,i,k}$	Unit capital investment of transportation mode k transporting freshwater from freshwater source s to shale site i
lc_i	NGL composition in shale gas at shale site i
$lfs_{s,i}$	Distance from freshwater source s to shale site i
lo_o	Recovery factor for treating wastewater of onsite treatment technology o
$lpm_{p,m}$	Distance from processing plant p to power plant m
$lpu_{p,u}$	Distance from processing plant p to underground reservoir u
$lsc_{i,c}$	Distance from shale site i to CWT facility c
$lsd_{i,d}$	Distance from shale site i to disposal well d
$lsp_{i,p}$	Distance from shale site i to processing plant p
$lum_{u,m}$	Distance from underground reservoir u to power plant m
mc_i	Methane composition in shale gas at shale site i
mn_i	Maximum number of wells that can be drilled at shale site i per time period
ocl_o	Minimum treatment capacity for onsite treatment technology o
ocu_o	Maximum treatment capacity for onsite treatment technology o
pci	Chemical engineering plant cost index
pcl	Minimum capacity of processing plant
pcu	Maximum capacity of processing plant
pef	Processing efficiency of shale gas
pl_t	Average unit price of NGL in time period t
psc_p	Minimum storage capacity of NGL for each time period at processing plant p
rcp	Reference capital investment for processing plant

rf_o	Ratio of freshwater to wastewater required for blending after treatment of onsite treatment technology *o*
rpc	Reference capacity of processing plant
$rpci_{pl}$	Chemical engineering plant cost index of the reference year for pipeline
$rpci_{pp}$	Chemical engineering plant cost index of the reference year for processing plant
$sdc_{i,t}$	Unit cost for shale well drilling and completion at shale site *i* in time period *t*
sfp	Size factor of processing plant
sft	Size factor of pipeline transporting shale gas and natural gas
smm	Reference capacity of pipeline transporting natural gas
smp	Reference capacity of pipeline transporting shale gas
$spc_{i,t}$	Unit cost for shale gas production at shale site *i* in time period *t*
$spp_{i,\tau}$	Shale gas production of a shale well of age τ at shale site *i*
srm	Reference capital investment of pipeline transporting natural gas
srp	Reference capital investment of pipeline transporting shale gas
$tcc_{i,c,k}$	Transportation capacity for transportation mode *k* from shale site *i* to CWT facility *c*
$tdc_{i,d,k}$	Transportation capacity for transportation mode *k* from shale site *i* to disposal well *d*
$tmcl$	Minimum capacity of pipeline transporting natural gas
$tmcu$	Maximum capacity of pipeline transporting natural gas
tmn_i	Maximum number of wells that can be drilled at shale site *i* over the planning horizon
$tpcl$	Minimum capacity of pipeline transporting shale gas
$tpcu$	Maximum capacity of pipeline transporting shale gas
$tsc_{s,i,k}$	Transportation capacity for transportation mode *k* from source *s* to shale site *i*
uca_u	Working gas capacity of underground reservoir *u*
ue	Amount of electricity generated per unit natural gas input
uic_u	Injection capability for each time period of underground reservoir *u*

uwc_u	Withdrawal capability for each time period of underground reservoir *u*
vc_c	Unit cost for wastewater treatment at CWT facility *c*
vd_d	Unit cost for underground injection of wastewater at disposal well *d*
ve_m	Unit cost for electricity generation from natural gas at power plant *m*
vo_o	Unit cost for wastewater treatment of onsite treatment technology *o*
vp	Unit processing cost for shale gas
vs	Unit storage cost for NGL
$vtcf_k$	Unit variable transportation cost for transportation mode *k* transporting freshwater
$vtcm$	Unit variable transportation cost for pipeline transporting natural gas
$vtcs$	Unit variable transportation cost for pipeline transporting shale gas
$vtcw_k$	Unit variable transportation cost for transportation mode *k* transporting wastewater
vui_u	Unit injection cost at underground reservoir *u*
vuw_u	Unit withdrawal cost at underground reservoir *u*
wd_i	Average drilling water usage for each well at shale site *i*
wrd_i	Recovery ratio of water for drilling process at shale site *i*
wrf_i	Recovery ratio of water for hydraulic fracturing process at shale site *i*

Continuous Variables

$FDW_{i,t}$	Freshwater demand of shale site *i* in time period *t*
$FW_{s,i,k,t}$	Amount of freshwater acquired from source *s* at shale site *i* using transportation mode *k* in time period *t*
$GE_{m,t}$	Amount of electricity generated at power plant *m* in time period *t*
$NN_{i,t}$	Number of wells drilled at shale site *i* in time period *t*
PC_p	Processing capacity for processing plant *p*
$PLS_{p,t}$	Amount of NGL sold at processing plant *p* in time period *t*
$SP_{i,t}$	Shale gas production rate at shale site *i* in time period

$SPL_{p,t}$ Amount of NGL produced at processing plant *p* in time period *t*

$SPM_{p,t}$ Amount of natural gas produced at processing plant *p* in time period *t*

$SPS_{p,t}$ Amount of NGL stored at processing plant *p* in time period *t*

$STP_{i,p,t}$ Amount of shale gas transported from shale site *i* to processing plant *p* in time period *t*

$STPM_{p,m,t}$ Amount of natural gas transported from processing plant *p* to power plant *m* in time period *t*

$STPU_{p,u,t}$ Amount of natural gas transported from processing plant *p* to underground reservoir *u* in time period *t*

$STUM_{u,m,t}$ Amount of methane transported from underground reservoir *u* to power plant *m* in time period *t*

$TCP_{i,p}$ Transportation capacity of pipeline from shale site *i* to processing plant *p*

$TCPM_{p,r}$ Transportation capacity of pipeline from processing plant *p* to power plant *m*

$TCPU_{p,u}$ Transportation capacity of pipeline from processing plant *p* to underground reservoir *u*

$TCUM_{u,m}$ Transportation capacity of pipeline from underground reservoir *u* to power plant *m*

$URS_{u,t}$ Amount of natural gas stored at underground reservoir *u* in time period *t*

$WP_{i,t}$ Wastewater production rate at shale site *i* in time period *t*

$WTC_{i,c,k,t}$ Amount of wastewater transported from shale site *i* to CWT facility *c* with transportation mode *k* for treatment in time period *t*

$WTD_{i,d,k,t}$ Amount of wastewater transported from shale site *i* to disposal well *d* with transportation mode *k* for injection in time period *t*

$WTO_{i,o,t}$ Amount of wastewater treated by onsite treatment technology *o* at shale site *i* in time period *t*

Binary Variables

$XC_{i,c,k}$	0-1 variable. Equal to 1 if transportation mode *k* is installed to transport water from shale site *i* to CWT facility *c*
$XD_{i,d,k}$	0-1 variable. Equal to 1 if transportation mode *k* is installed to transport water from shale site *i* to disposal well *d*
$XP_{i,p}$	0-1 variable. Equal to 1 if pipeline is installed to transport shale gas from shale site *i* to processing plant *p*
$XPM_{p,m}$	0-1 variable. Equal to 1 if pipeline is installed to transport natural gas from processing plant *p* to power plant *m*
$XPU_{p,u}$	0-1 variable. Equal to 1 if pipeline is installed to transport natural gas from processing plant *p* to underground reservoir *u*
$XUM_{u,m}$	0-1 variable. Equal to 1 if pipeline is installed to transport natural gas from underground reservoir *u* to power plant *m*
$XS_{s,i,k}$	0-1 variable. Equal to 1 if transportation mode *k* is installed to transport fresh water from source *s* to shale site *i*
$YO_{i,o}$	0-1 variable. Equal to 1 if onsite treatment technology *o* is applied at shale site *i*
YP_p	0-1 variable. Equal to 1 if processing plant *p* is set up
$YD_{i,n,t}$	0-1 variable. Equal to 1 if *n* shale wells at shale site *i* are drilled in time period *t*

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