

Optimal Design and Operations of Supply Chain Networks for Water Management in Shale Gas Production: MILFP Model and Algorithms for the Water-Energy Nexus

Jiyao Gao and Fengqi You

Dept. of Chemical and Biological Engineering, Northwestern University, Evanston, IL 60208, USA

DOI 10.1002/aic.14705

Published online December 21, 2014 in Wiley Online Library (wileyonlinelibrary.com)

The optimal design and operations of water supply chain networks for shale gas production is addressed. A mixed-integer linear fractional programming (MILFP) model is developed with the objective to maximize profit per unit freshwater consumption, such that both economic performance and water-use efficiency are optimized. The model simultaneously accounts for the design and operational decisions for freshwater source selection, multiple transportation modes, and water management options. Water management options include disposal, commercial centralized wastewater treatment, and onsite treatment (filtration, lime softening, thermal distillation). To globally optimize the resulting MILFP problem efficiently, three tailored solution algorithms are presented: a parametric approach, a reformulation-linearization method, and a novel Branch-and-Bound and Charnes–Cooper transformation method. The proposed models and algorithms are illustrated through two case studies based on Marcellus shale play, in which onsite treatment shows its superiority in improving freshwater conservancy, maintaining a stable water flow, and reducing transportation burden. © 2014 American Institute of Chemical Engineers AIChE J, 61: 1184–1208, 2015

Keywords: supply chain optimization, water management, MINLP, shale gas, Branch-and-Bound

Introduction

Natural gas is playing a significant role in meeting global energy demand, and is also serving as a transition fuel as the U.S. develops more sustainable fuel options. Shale gas is unconventional natural gas extracted from shale rock and has emerged as one of the most promising energy sources within the past decade. In 2012, 35% of the U.S. natural gas production was from shale gas.^{1,2} The U.S. shale gas reserves were estimated to be 482 trillion cubic feet in a June 2012 study.³ With increasing production of shale gas, the U.S. has changed from an importer to a net exporter of natural gas.^{4,5} The recent large-scale production of shale gas would not have been possible without the development of hydraulic fracturing and horizontal drilling technologies.^{6,7} During hydraulic fracturing, millions of gallons of fracturing fluid (mainly water) is pumped into the wellbore with high pressure, fracturing the rock layer and increasing the production rate of oil and/or gas. Horizontal drilling allows for the drilling of multiple horizontal wellbores in a shale site, reducing the capital investment and improving the efficiency of shale gas production.⁸ The combined application of hydraulic fracturing and horizontal drilling technologies has led to an exponential increase of shale gas production.^{9–11}

Despite the economic potential of using hydraulic fracturing and horizontal drilling technologies for shale gas production, there are increasing concerns about water consumption.^{10,12–16} It is known that the hydraulic fracturing operation during the shale gas production process requires a significant amount of freshwater, accounting for 90% of the overall water usage.¹⁷ In 2006, about 35,000 shale wells were drilled in the U.S., and each well required approximately 4–6 million gallons of injected water for shale gas production.^{18–21} Meanwhile, in shale plays such as Marcellus, 10–25% of the injected water flows back to the surface as highly contaminated water. Depending on the specific region, this range may vary significantly. This water contains a high concentration of total dissolved solids (TDS) as well as other toxic and radioactive dissolved constituents.^{22,23} This wastewater is challenging and costly to treat. Economical production of shale gas requires effective wastewater management to minimize freshwater consumption while ensuring sufficient water supply to fracturing operations. Due to different water flow rates and water compositions in the shale wells, it is very important to determine the corresponding optimal strategies for water management.

An overview of the water management problem for shale gas production is depicted in Figure 1. Water from freshwater sources, which is mainly surface water from rivers or lakes, is transported to shale sites by pipeline or truck. There are some alternative freshwater sources, including groundwater, treated wastewater, cooling water, and so forth. At shale sites, fracturing fluid is prepared, which mainly consists of water (over 90%), sand (9%), and chemical additives (0.5%).²⁴ This fracturing fluid is pumped into the wellbore at a high pressure.

Contract grant sponsor: Institute for Sustainability and Energy at Northwestern University (ISEN).

Correspondence concerning this article should be addressed to F. You at you@northwestern.edu.

© 2014 American Institute of Chemical Engineers

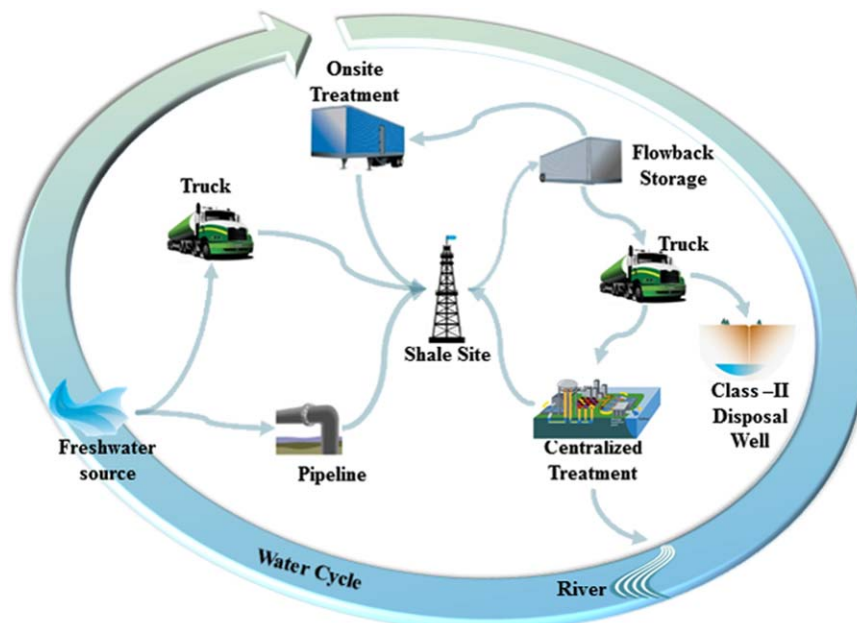


Figure 1. Overview of water management for shale gas production.

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

Meanwhile, a certain amount of the injected fracturing fluid returns to the surface as wastewater, containing dissolved salts, minerals, residual fracturing fluid additives, heavy metals, bacteria, suspended solids, naturally occurring radioactive material, volatile organics, hydrocarbons, and ammonia.^{14,24} The water that flows back can be classified by the amount of TDS per liter. Based on the operational definition, water produced during the well completion stage is defined as flowback water; meanwhile water is referred to as produced water when the well is under production. Normally, the volumetric flow rate of flowback water is significantly larger than that of produced water, and the produced water tends to have higher concentration of TDS, likely because of its longer residence time downhole as well as a smaller flow rate. As a whole, we can observe the flow rate of wastewater decreases along with time while the salinity of wastewater increases with time.^{25,26} The resulting wastewater can be temporarily stored in tanks or impoundments, transported to Class-II disposal wells for underground injection, transported to commercial centralized wastewater treatment (CWT) facilities for treatment, or directly treated by onsite treatment facilities for reuse.^{14,25,27} Multiple technologies are involved in each of these water management options, which are explicitly introduced in the Background Section.

Most existing work on this topic focus on the shale gas production process, including the design and operations of shale gas supply chains,²⁸ regulations on shale gas production,²⁹ transportation technologies,³⁰ emission of shale gas,³¹ and other aspects.^{32,33} With the rapid development of hydraulic fracturing in recent years, there is an increasing concern regarding freshwater consumption and wastewater disposal. Existing publications in this area focus on the environmental impacts of hydraulic fracturing,^{34–36} or on the technoeconomic analysis and optimization of specific water management options,^{25,37} and water consumption is considered as an important issue for shale gas production.^{15–17} The recently published report by the U.S. Department of Energy emphasized that water scarcity, variability, and uncertainty

are becoming more prominent, potentially leading to vulnerabilities of the U.S. energy system. Thus, it is imperative to develop a more integrated approach to address the challenges and opportunities of the water-energy nexus in shale gas production.³⁸ Yang et al.¹⁴ recently proposed a two-stage stochastic mixed-integer linear programming (MILP) model that optimizes water-use life cycle in hydraulic fracturing. However, they only focused on the operational scheduling problem without considering the strategic design decisions. Moreover, they solely optimize the economic (cost/profit) objective by dividing the whole network into freshwater handling section and wastewater handling section. Therefore, the goal of this work is to develop a modeling and optimization framework for integrated design and operations of a water supply chain network for shale gas production, with explicit consideration of multiple water management options and corresponding technologies, as well as the tradeoff between cost effectiveness and freshwater conservancy.

To achieve this goal, there are several challenges that need to be addressed. The first challenge is the simultaneous optimization of the economic performance and freshwater consumption in the integrated supply chain optimization model. Another challenge is accounting for various water management options (e.g., injection into Class-II disposal wells, CWT facilities, and different levels of onsite treatments) in a comprehensive optimization model. We note that these water management options, as well as the diverse water treatment technologies, have their advantages and limitations. A third challenge is modeling the relationship between the composition of wastewater and the input/output of the water management options. Finally, the last challenge involves effectively solving the resulting optimization problem, especially for large-scale applications.

In this work, we propose a novel mixed-integer linear fractional programming (MILFP) model for the optimal design and operations of water supply chain networks for shale gas production. We consider a fractional function as the objective, the numerator of which is the profit for shale

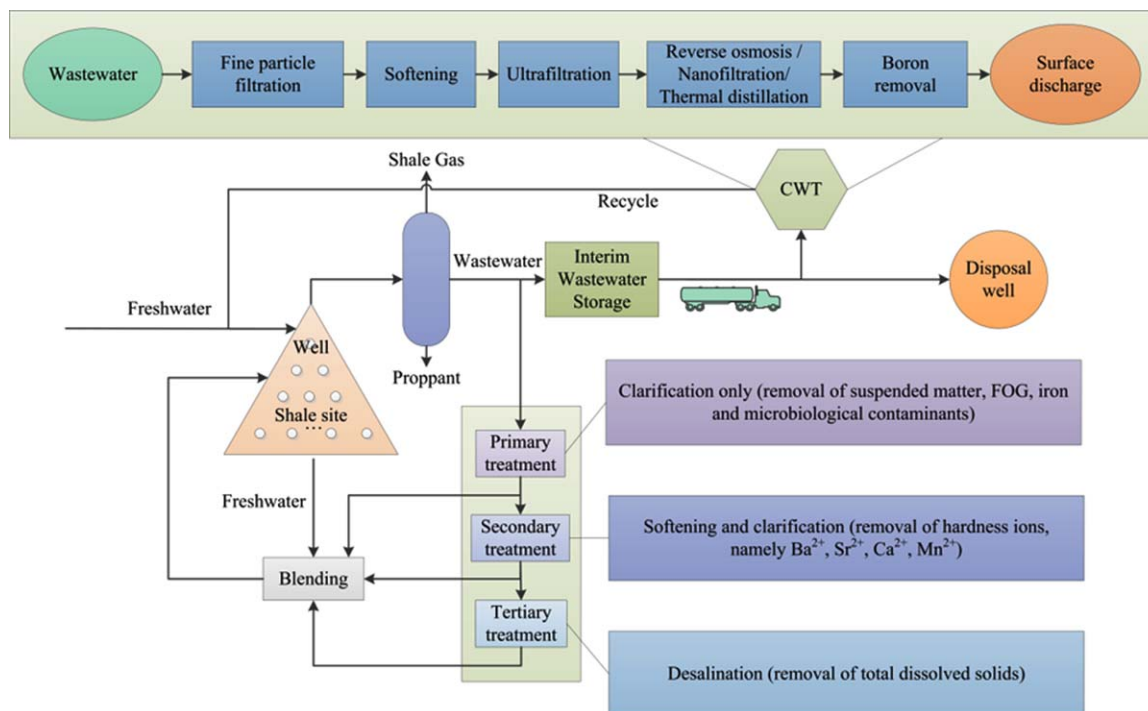


Figure 2. Illustration of water management options and the corresponding treatment technologies.

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

gas production and the denominator is the net freshwater consumption. This objective function reflects the profit associated with unit net consumption of freshwater. The model takes into account both strategic design and operational planning decisions of water supply chain networks for shale gas production. The design decisions include the selection of freshwater sources, water transportation modes, and onsite treatment technologies, as well as the capacity of water treatment facilities. The operational decisions include the amount of freshwater delivered from each water source to each shale site, as well as the amount of wastewater transported to each disposal well, stored temporarily onsite, treated by each CWT facility or onsite treatment facility, and reused in each shale site at each time period. Due to the presence of the fractional objective and discrete variables, the resulting MILFP problem, which is within a class of nonconvex mixed-integer nonlinear programming (MINLP) problems, can be computationally intractable for large-scale instances. To facilitate the solution process, we present three tailored global optimization algorithms: a parametric algorithm based on the exact Newton's method, a reformulation-linearization method, and a novel algorithm integrating the Branch-and-Bound and Charnes–Cooper transformation methods. We present two case studies to demonstrate the proposed optimization model and algorithms. In the first small-scale case study, we compare the optimization results obtained using two different objective functions, that is, the proposed fractional objective and a linear one minimizing the total supply chain cost. In the second large-scale case study based on Marcellus shale play, we optimize the design and operation of a water supply chain network including up to 10 freshwater sources, 10 shale sites with 10 shale wells per site, 5 CWT facilities, and 50 disposal wells over a 10-year planning horizon with 520 time periods.

The major novelties of this work are summarized as follows:

- A novel MILFP model that simultaneously optimizes the economic performance and water-use efficiency in the design and operations of water supply chain networks for multisite shale gas production.
- A novel global optimization algorithm that combines standard Branch-and-Bound algorithm with Charnes–Cooper transformation for solving general MILFP problems.
- An illustrative small-scale case study and a large-scale case study based on Marcellus shale play to illustrate the application of the proposed modeling and optimization framework.

The rest of this article is organized as follows. A brief background on the different water management options is provided in the “Background” section. It is followed by the problem statement and the optimization model formulation. Two tailored algorithms and the novel Branch-and-Bound and Charnes–Cooper transformation method for solving MILFP are introduced in the “Solution Approaches” section. To illustrate the application, one illustrative small-scale case study and one large-scale case study based on Marcellus shale play are presented at the end of the manuscript.

Background on Water Management Options

There are three main water management options: direct injection into the Class-II disposal wells, commercial CWT for surface discharge, and onsite treatment for reuse in hydraulic fracturing operations. A flow diagram of these water management options is depicted in Figure 2.

The first option is injection into Class-II disposal wells. Disposal wells for injection of brine associated with oil and gas operations are classified as Class II in US Environmental Protection Agency's Underground Injection Control

program.^{25,27} In the following content, we use disposal wells to indicate the Class-II disposal wells. As can be seen from Figure 2, after the extraction of shale gas and intermediate storage, the untreated wastewater is directly sent to disposal wells and pumped into deep, impermeable rock layers. Injection in disposal wells is often chosen when nearby disposal wells are available for underground injection of wastewater. For States where there are abundant disposal wells, namely Texas, the underground injection options is considered as a cost-effective water management option; while for states such as Pennsylvania, which is reported to have only eight disposal wells with limited available capacity,³⁹ wastewater from Marcellus drilling must be transported to out-of-state locations, namely Ohio, for disposal, making underground injection less attractive due to high transportation cost.⁴⁰ As there is no water treatment process involved for injection disposal, the disposal wells option might become economically appealing for wastewater that is difficult and expensive to treat. However, in some regions, there might not be suitable disposal wells, or there are regulations restricting the usage of disposal wells. In addition, there are concerns on the risks of underground water contamination and induced seismicity by injecting wastewater from hydraulic fracturing into disposal wells, thus, the amount of wastewater injected underground must subject to the available capacity of disposal wells.^{18,36} When the option of disposal well injection is not locally available, wastewater might need to be trucked over a long distance to disposal wells located in other regions, possibly rendering this option uneconomical.

The second option is the commercial wastewater treatment facilities, or CWT facilities, which are capable of treating flowback and produced water. The treated water is then discharged to surface water bodies or recycled to shale sites for reuse. The resulting concentrated brine from these treating processes is all going to injection or taken down to zero-liquid discharge condition and disposed of as solid waste, which is not considered in this model.^{19,39} As shown in Figure 2, wastewater from shale sites is transported to CWT facilities and treated with a sequence of treatment technologies. We note that the specific technologies used in CWTs might differ from those presented here, but the given technologies, such as reverse osmosis and thermal distillation technologies are all common options applied in commercial wastewater treatment.^{24,26,27,41} For a general CWT facility, the first step is fine particle filtration where the wastewater is first screened to remove large objects and then pumped into a settling tank to allow settling of heavy solids and removal of any free oil. The second step is softening, where wastewater goes through several processes including agitation, aeration, and pH adjustment with lime to soften the water. The third step is ultrafiltration, where particulates and macromolecules are removed. The following step is reverse osmosis/nanofiltration/thermal distillation, where most salts and other effluent materials except water are removed. Lastly, certain toxic elements such as boron need to be removed to meet the specifications of surface discharge or reuse.²⁷ After these treatment processes, the treated water can be recycled to shale sites or directly sent to surface discharge. In other words, the recycled water can be reused for hydraulic fracturing again, and the discharged water returns to the natural water cycle and does not contribute to net freshwater consumption. Thus, a major advantage of this option is that it can help reduce the freshwater consumption. Moreover, CWT facilities

generally have a lower treatment cost than that of onsite treatment options because of their large operating capacities and economies of scale. However, due to transportation costs, the economic viability of this water management option might be affected by the proximity of these CWT facilities to shale sites. Generally, water treatment facilities cannot recover all the treated water, so part of the treated water is lost during the treating process.²⁴

The last option is onsite treatment for reuse. The onsite treatment is usually performed by some commercial water treatment companies, each of them may include different treatment technologies.^{27,42} As shown in Figure 2, wastewater can be treated by three levels of onsite water treatment technologies. The treated water is blended with a certain amount of freshwater to satisfy the specifications of reuse and then flows back to the shale site for hydraulic fracturing. The three levels of onsite treatments include the primary, secondary, and tertiary treatment.²⁴ We note that for the primary and secondary onsite treatment, water is partially treated, and a certain amount of make-up water is required for blending to reduce the TDS concentration to satisfy the reuse specification. For tertiary treatment, a certain amount of make-up water is required to blend with the wastewater to reduce the TDS concentration of the wastewater, so that it can be treated effectively by multiple desalination technologies.^{27,43}

- Primary treatment involves clarification only, where suspended matter, free oil and grease (FOG), iron, and microbiological contaminants are removed. There are multiple technologies for primary treatment, including coagulation, flocculation and disinfection, electrocoagulation, disinfection, microfiltration/ultrafiltration, adsorption, ozonation, and use of a hydrocyclone.

- Secondary treatment, based on the simple clarification process, mainly involves softening, where hardness ions such as Ba^{2+} , Sr^{2+} , Ca^{2+} , and Mn^{2+} are removed. Secondary treatment technologies include lime softening, ion exchange, and activated carbon.

- Tertiary treatment, in addition to the clarification and softening process, focuses on desalination, which mainly removes the TDS. Generally, there are four kinds of technologies for desalination: membrane separation, electrically driven membrane separation, thermal technologies, and zero-liquid discharge. Membrane separation technologies include nanofiltration, reverse osmosis, forward osmosis, and membrane distillation. Capacitive deionization and electrodialysis reversal technologies are typical technologies of electrically driven membrane separation. Thermal technologies include multieffect distillation, multistage flash, and vapor compression. Crystallization and evaporator/concentrator are typical zero-liquid-discharge technologies.

As treated water can be blended with a certain percentage of freshwater to satisfy the reuse specification, water treated onsite can be reused for hydraulic fracturing. The onsite treatment option can help reduce the net freshwater consumption directly. Moreover, as the wastewater is directly handled by onsite treatment facilities, there is no transportation cost involved. However, onsite treatment is limited by capacity and technical constraints, and its economic efficiency highly depends on the wastewater composition and the treatment technology applied. For example, water with a relatively low TDS concentration can be treated simply by primary treatment, such as filtration and blending. However,

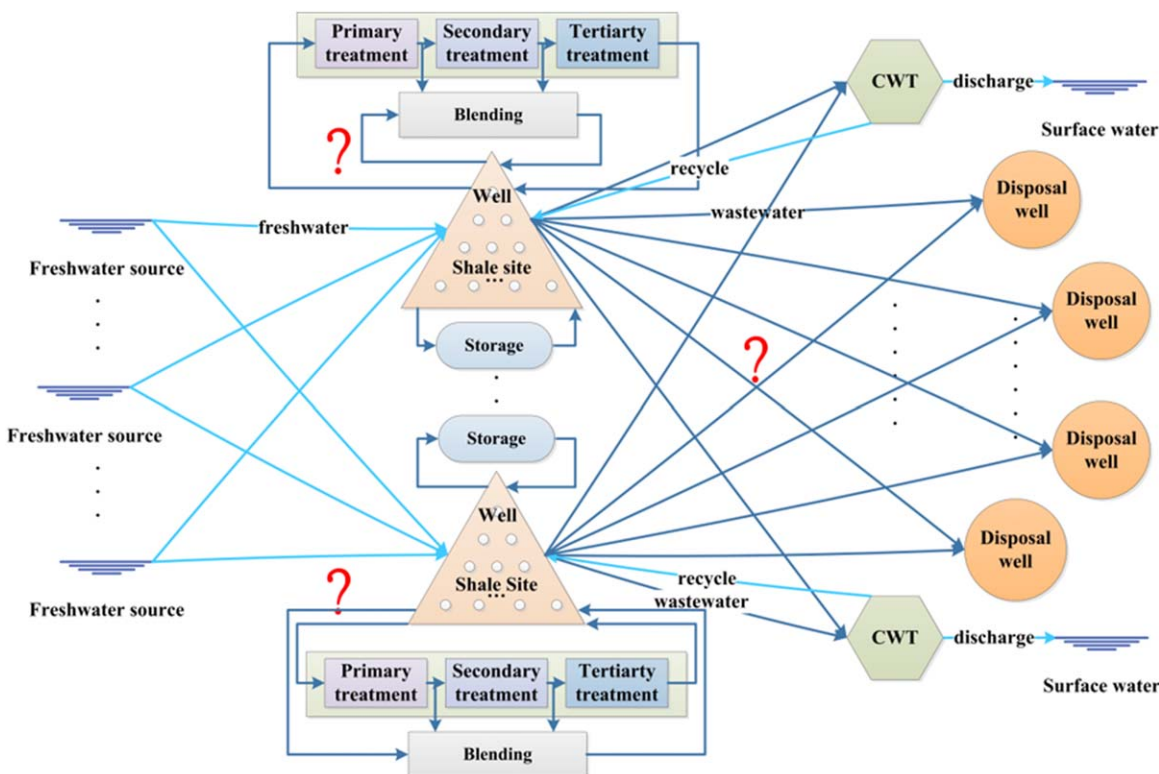


Figure 3. Superstructure of the water supply chain for shale gas production.

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

water with a high TDS concentration can only be treated by cost or energy-intensive technologies, for example, thermal distillation for tertiary treatment.⁴³ Similar to the CWT option, there is also an inevitable loss of water for onsite treatment, depending on both the composition of water and the exact treatment technology.

Apart from these three water management options, wastewater can be stored temporarily at the shale sites within tanks or impoundments.^{44,45} Generally, the storage capacity of wastewater for each shale site is limited. The wastewater storage option functions like inventory that can provide “buffer” for transportation or treatment activities across the time periods.

Problem Statement

In this section, we formally state the problem of optimal design and operations of water supply chain networks for shale gas production.

We consider the following assumptions for this problem:

- Profit from shale gas production is considered as known parameter in this work.¹⁴
- All the capital investment decisions are made at the beginning of project.
- The differences in freshwater composition from different water sources can be neglected.
- Time delays due to water treatment, production, or transportation can be neglected compared with the long-term strategic planning horizon.

We address the problem over a planning horizon divided into a set of time periods with identical intervals. This model includes a set of shale sites with multiple wells at each site. During the shale gas production process, these

shale sites need freshwater for drilling and hydraulic fracturing. They can get water from different freshwater sources by different transportation modes. Meanwhile, wastewater is generated during shale gas production. The volume and TDS concentration of the wastewater vary with location and time. Wastewater produced during the well completion stage, that is, the drilling process, has a large flow rate but fewer TDS. This drilling process is defined as the first 4 weeks after fracturing, which approximately equals to the drilling time of shale well.¹⁷ Later when the shale well is considered to be under production, it is considered to be the hydraulic fracturing process, and the corresponding water has a much lower flow rate and a higher TDS concentration.^{17,43} To handle the wastewater, we have the following options:

- Stored onsite temporarily in tanks or impoundments for future disposal or treatment;
- Transported to existing commercial CWT facilities for treatment and then go to surface discharge or recycling;
- Transported to existing available Class-II disposal wells for direct underground injection;
- Treated through three levels of onsite treatment units and blended with a certain amount of freshwater for reuse.

Three levels of onsite treatments are considered: primary, secondary, and tertiary treatment. For each level of onsite treatment, we are given a set of water treatment technology options. Water is classified into a set of TDS concentration ranges according to its TDS concentration.

A general water supply chain superstructure is given in Figure 3. The network includes a set of freshwater sources, a set of shale sites, a set of wells in each shale site, a set of CWT facilities and disposal wells, a set of transportation links, and a set of transportation modes for each

transportation link, as well as different levels of potential onsite treatment facilities for each shale site. In this problem, we are given the following parameters,

- Unit cost and capacity of water supply at each freshwater source;
- Demand of water, number of wells, production profile of wastewater, initial storage capacity, correlation between shale gas production and wastewater generation, and average revenue for unit shale gas production at each shale site;
- Unit operating cost, capacity, and recovery factor for treating wastewater with different TDS concentration at each CWT facility;
- Unit operating cost and capacity at each disposal well;
- Capital investment, unit operating cost, recovery factor, capability of treating different TDS concentration ranges wastewater, and percentage of freshwater required for blending at each onsite treatment facility;
- Capital investment as well as unit operating cost for each transportation mode of every transportation link.

Major decision variables for this problem are summarized as follows:

- Selection of freshwater sources;
- Amount of freshwater transported by each transportation mode from each freshwater source to each shale site;
- Amount of wastewater injected in disposal wells for each shale site;
- Amount of wastewater treated by CWT facilities for discharge or recycling for each shale site;
- Amount of wastewater treated by different onsite treatment technologies at each shale site;
- Amount of wastewater stored temporarily onsite at each shale site at each time period.
- Selection of transportation modes and corresponding transportation flow;
- Capacity of each transportation mode for each transportation link;
- Capacity of onsite treatment facilities to be installed at each shale site.

The objective of this problem is to maximize the profit per unit freshwater consumption. The goal is to seek a balance between cost effectiveness and freshwater conservancy. To illustrate the benefit of such a fractional objective function, a comparison between this fractional objective function and a linear objective function is given in the Case Studies section.

Model Formulation

According to the general problem statement in the previous section, we present the model formulation for the optimal design and operations of water supply chain networks for shale gas production. A list of indices, sets, parameters, and variables is given in the Notation, where all the parameters are denoted with upper-case symbols and all the variables are denoted with lower-case symbols. In the following subsection, constraints in the proposed models are presented.

Constraints

The total water demand is satisfied by freshwater and reused water from onsite treatment. Thus, the mass balance relationship of the water supply is given by

$$\sum_{s \in S} \sum_{m \in M} fw_{s,i,m,t} + \sum_{c \in C} \sum_{m \in M} wtr_{i,c,m,t} + \sum_{l \in L} \sum_{o \in O} LO_{l,o} \cdot wto_{i,l,o,t} = \sum_{j \in J} RW_{i,j,t}, \forall i, t \quad (1)$$

The first term denotes the total freshwater from all the water sources to shale site i at time period t . $fw_{s,i,m,t}$ denotes the amount of freshwater transported by transportation mode m from freshwater source s to shale site i at time period t . The second term denotes the recycled water from CWT facilities to shale site i at time period t , $wtr_{i,c,m,t}$ denotes the amount of treated water at CWT facility c recycled to shale site i with transportation mode m at time period t . The third term is the water being treated onsite and reused at shale site i at time period t . $LO_{l,o}$ is the recovery factor for TDS concentration range l water treated by level o onsite treatment; $wto_{i,l,o,t}$ stands for the amount of TDS concentration range l water treated by level o onsite treatment at time period t ; $RW_{i,j,t}$ on the right hand side is the water demand for fracturing at shale site i at time period t .

At each shale site, the total newly produced wastewater from all wells together with the wastewater stored onsite at the previous time period should equal the total water flow with respect to different water management options including CWT, disposal, onsite treatment, and onsite storage. This output flow balance relationship for the waste water is given by

$$\sum_{j \in J} WP_{i,j,l,t} + ws_{i,l,t-1} = \sum_{c \in C} \sum_{m \in M} wic_{i,l,c,m,t} + \sum_{o \in O} wto_{i,l,o,t} + ws_{i,l,t}, \forall i, t \quad (2)$$

where $WP_{i,j,l,t}$ denotes the production amount of TDS concentration range l wastewater at shale site i at time period t ; $wic_{i,l,c,m,t}$ denotes the amount of TDS concentration range l water at shale site i transported by transportation mode m to CWT facility c for treatment at time period t ; $wtd_{i,l,d,m,t}$ denotes the amount of TDS concentration range l water at shale site i transported by transportation mode m and injected in disposal well d at time period t ; $ws_{i,l,t}$ denotes the amount of TDS concentration range l water stored at shale site i at time period t .

At each CWT facility, the treated water can either be disposed directly to surface water bodies or recycled to shale sites for reuse

$$\sum_{i \in I} \sum_{l \in L} \sum_{m \in M} LC_l \cdot wtr_{i,l,c,m,t} = wtd_{c,t} + \sum_{i \in I} \sum_{m \in M} wtr_{i,c,m,t}, \forall c, t \quad (3)$$

where LC_l denotes the recovery factor for the CWT facility treating TDS concentration range l of water. $wtd_{c,t}$ denotes the amount of treated water at CWT facility c disposed directly to surface water at time period t .

The total freshwater supply from each freshwater source to all the shale sites by trucks and by pipelines should not exceed the supply capacity of this freshwater source, given by

$$\sum_{i \in I} \sum_{m \in M} fw_{s,i,m,t} \leq FR_{s,t}, \forall s, t \quad (4)$$

where $FR_{s,t}$ denotes the capacity of freshwater source s at time period t .

The amount of freshwater transported by transportation mode m from freshwater source s to shale site i is constrained by the total capacity of transportation mode m with different capacity ranges, given by

$$fw_{s,i,m,t} \leq \sum_{r \in R} tsc_{s,i,m,r}, \forall s, i, m, t \quad (5)$$

where $tsc_{s,i,m,r}$ denotes the capacity of transportation mode m from freshwater source s to shale site i with capacity range r .

The amount of wastewater transported by transportation mode m from shale site i to CWT facility c cannot exceed the total capacity of transportation mode m with different capacity ranges, given by

$$\sum_{l \in L} wtc_{i,l,c,m,t} \leq \sum_{r \in R} tcc_{i,c,m,r}, \forall i, c, m, t \quad (6)$$

where $tcc_{i,c,m,r}$ denotes the capacity of transportation mode m from shale site i to CWT facility c with capacity range r .

The amount of wastewater transported by transportation mode m from shale site i to disposal well d is bounded by the total capacity of transportation mode m with different capacity ranges given by

$$\sum_{l \in L} wtd_{i,l,d,m,t} \leq \sum_{r \in R} tdc_{i,d,m,r}, \forall i, d, m, t \quad (7)$$

where $tdc_{i,d,m,r}$ denotes the capacity of transportation mode m from shale site i to disposal well d with capacity range r .

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

$$\sum_{i \in I} \sum_{l \in L} \sum_{m \in M} wtc_{i,l,c,m,t} \leq WC_{c,t}, \forall c, t \quad (8)$$

where $WC_{c,t}$ denotes the capacity of CWT facility c at time period t .

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

$$\sum_{i \in I} \sum_{l \in L} \sum_{m \in M} wtd_{i,l,d,m,t} \leq WD_{d,t}, \forall d, t \quad (9)$$

where $WD_{d,t}$ denotes the capacity of disposal well d at time period t .

The amount of water treated onsite is bounded by the capacities of onsite treatment facilities

$$wto_{i,l,o,t} \leq \sum_{q \in Q} oc_{i,l,o,q}, \forall i, l, t, \quad o \in O(l) \quad (10)$$

where $oc_{i,l,o,q}$ denotes the capacity of level o onsite treatment facility with capacity range q for treating TDS concentration range l water at shale site i ; $O(l)$ is the subset of onsite treatments that are capable of treating TDS concentration range l water.

The total amount of water stored onsite at each shale site at each time period cannot exceed the total storage capacity at that site, given by

$$\sum_{l \in L} ws_{i,l,t} \leq SC_i + sca_i, \forall i, t \quad (11)$$

where SC_i stands for the initial impoundments storage capacity at shale site i , and sca_i denotes the additional tanks

storage capacity that can be installed at shale site i in the beginning of project, which requires extra capital investment.

The additional storage capacity that can be installed at each shale site is limited, given by

$$sca_i \leq SM_i, \forall i \quad (12)$$

where SM_i denotes the maximum additional storage capacity that can be installed at shale site i .

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

$$\sum_{l \in L} \sum_{o \in O} RF_o \cdot LO_{l,o} \cdot wto_{i,l,o,t} \leq \sum_{s \in S} \sum_{m \in M} fw_{s,i,m,t} + \sum_{c \in C} \sum_{m \in M} wtc_{i,c,m,t}, \forall i, t \quad (13)$$

where RF_o is the ratio of freshwater to wastewater required for blending after level o onsite treatment; $LO_{l,o}$ stands for the recovery factor for level o onsite treatment treating TDS concentration range l water.

All the bounding constraints with respect to constructions of transportation mode m and onsite treatment facilities are given as follows. If transportation mode m is installed between freshwater source s to shale site i , its freshwater transportation amount cannot exceed the availability of corresponding freshwater source; otherwise, the transportation amount should be zero. We note that the capacity of each transportation mode is classified into a set of capacity ranges, indexed by r

$$fw_{s,i,m,t} \leq \sum_{r \in R} xs_{s,i,m,r} \cdot FR_{s,t}, \forall s, i, m, t \quad (14)$$

where binary variable $xs_{s,i,m,r}$ is introduced to determine the installation of transportation mode m between water source s and shale site i . If $xs_{s,i,m,r} = 1$, transportation mode m with capacity range r is installed between water source s and shale site i ; otherwise not installed.

Similarly, if transportation mode m is installed between shale site i and CWT facility c , its wastewater transportation amount cannot exceed the capacity of CWT facility c ; otherwise, the transportation amount should equal zero

$$wtc_{i,l,c,m,t} \leq \sum_{r \in R} xc_{i,c,m,r} \cdot WC_{c,t}, \forall i, l, c, m, t \quad (15)$$

where the binary variable $xc_{i,c,m,r}$ is used to determine the installation of transportation mode m between shale site i and CWT facility c . If $xc_{i,c,m,r} = 1$, transportation mode m with capacity range r is established between shale site i and CWT facility c ; otherwise it is not established.

If transportation mode m is established between shale site i and disposal well d , its wastewater transportation amount cannot exceed the capacity of disposal well d ; otherwise, the transportation amount would equal zero

$$wtd_{i,l,d,m,t} \leq \sum_{r \in R} xd_{i,d,m,r} \cdot WD_{d,t}, \forall i, l, d, m, t \quad (16)$$

where the binary variable $xd_{i,d,m,r}$ determines the establishment of transportation mode m between shale site i and disposal well d . If $xd_{i,d,m,r} = 1$, transportation mode m with capacity range r is available between shale site i and disposal well d ; otherwise, it is not available.

If transportation mode m is installed, its capacity should be bounded by the corresponding capacity ranges; otherwise, the capacity of transportation mode m should equal zero. Thus, we have the following constraints

$$MS_{s,i,m,r-1} \cdot x_{s,i,m,r} \leq tsc_{s,i,m,r} \leq MS_{s,i,m,r} \cdot x_{s,i,m,r}, \quad \forall s, i, m, r \quad (17)$$

where $MS_{s,i,m,r}$ denotes the maximum capacity of transportation mode m with capacity range r from source s to shale site i .

We have similar constraints for the capacity of transportation mode m from shale site i to CWT facility c , given by

$$MC_{i,c,m,r-1} \cdot x_{c,i,m,r} \leq tcc_{i,c,m,r} \leq MC_{i,c,m,r} \cdot x_{c,i,m,r}, \quad \forall i, c, m, r \quad (18)$$

where $MC_{i,c,m,r}$ stands for the maximum capacity of transportation mode m with capacity range r from shale site i to CWT facility c .

The constraints for the capacity of transportation mode m from shale site i to disposal well d are given by

$$MD_{i,d,m,r-1} \cdot x_{d,i,m,r} \leq tdc_{i,d,m,r} \leq MD_{i,d,m,r} \cdot x_{d,i,m,r}, \quad \forall i, d, m, r \quad (19)$$

where $MD_{i,d,m,r}$ indicates the maximum capacity of transportation mode m with capacity range r from shale site i to disposal well d .

If a certain onsite treatment facility is built up, its treatment capacity should be bounded by the corresponding capacity range; otherwise, the treatment capacity should be zero. This relationship can be modeled by the following inequality

$$WO_{i,o,q-1} \cdot y_{i,o,q} \leq \sum_{l \in L} oC_{i,l,o,q} \leq WO_{i,o,q} \cdot y_{i,o,q}, \quad \forall i, o, q \quad (20)$$

where the binary variable $y_{i,o,q}$ is used to determine the installation of onsite treatment facilities. If $y_{i,o,q} = 1$, a level o onsite treatment facility with capacity range q is installed at shale site i ; otherwise, this onsite treatment facility is not installed.

We specify that at most one capacity range for transportation mode m can be installed for each transportation link, including freshwater sources to shale sites, shale sites to CWT facilities and shale sites to disposal wells

$$\sum_{r \in R} x_{s,i,m,r} \leq 1, \quad \forall s, i, m \quad (21)$$

$$\sum_{r \in R} x_{c,i,m,r} \leq 1, \quad \forall i, c, m \quad (22)$$

$$\sum_{r \in R} x_{d,i,m,r} \leq 1, \quad \forall i, d, m \quad (23)$$

Similarly, at most one onsite treatment facility of capacity range level o can be installed at shale site i , given by

$$\sum_{q \in Q} y_{i,o,q} \leq 1, \quad \forall i, o \quad (24)$$

Objective functions

Fractional Objective Function of MILFP Model (P). In this water supply chain design and operations problem, we

first consider a model with a fractional objective that maximizes the profit per unit freshwater consumption. The resulting MILFP problem is denoted as (P), and the objective function is given by

$$\max \quad npf = \frac{NP - cw}{nf} \quad (25)$$

where NP denotes the profit of shale gas production excluding water management cost; cw denotes the total cost of the water supply chain network; and nf denotes the net freshwater consumption.

Linear Objective Function of MILP Model (EP). To demonstrate the advantage of this fractional objective function applied in problem (P), we consider another model for comparison, and the resulting problem is denoted as (EP). The objective of problem (EP) is a linear function maximizing the total profit of this water supply chain network. As a result, problem (EP) is an MILP problem with objective function given by

$$\max \quad NP - cw \quad (26)$$

There are a set of terms involved in objectives of (P) and (EP), which are given as follows.

The term NP stands for the total net present profit gained by shale gas production excluding the water management cost. We note it is a parameter here, which is calculated by

$$NP = \sum_{i \in I} \sum_{j \in J} \sum_{l \in L} \sum_{t \in T} \frac{SP_{i,t} \cdot WP_{i,j,l,t} \cdot CC_{i,j,t}}{(1+DR)^t} \quad (27)$$

where $SP_{i,t}$ denotes the average revenue per unit shale gas production at shale site i at time period t ; $WP_{i,j,l,t}$ denotes the TDS concentration range l wastewater production profile for well j at shale site i at time period t ; $CC_{i,j,t}$ is the correlation coefficient between water and shale gas production profiles for well j at shale site i at time period t ; and DR is the discount rate per time period.

The term cw stands for the total net present cost in the water supply chain, including the following items

$$cw = c_{\text{water}} + c_{\text{transport}} + c_{\text{handling}} \quad (28)$$

where c_{water} denotes the total net present cost for freshwater acquisition; $c_{\text{transport}}$ denotes the total net present cost for water transportation, including both freshwater and wastewater; and $c_{\text{treatment}}$ denotes the total net present cost for handling wastewater by different options. The detailed formulations for these terms are presented as follows:

The total net present cost for freshwater acquisition is given by

$$c_{\text{water}} = \sum_{s \in S} \sum_{i \in I} \sum_{m \in M} \sum_{t \in T} \frac{WA_s \cdot fw_{s,i,m,t}}{(1+DR)^t} \quad (29)$$

where WA_s denotes the unit freshwater acquisition cost from freshwater source s .

The total net present cost for water transportation is quantified by constraints (30)–(36), as the sum of freshwater transportation cost from freshwater sources to shale sites and the wastewater transportation cost from shale sites to CWT facilities or disposal wells. This is given by

$$c_{\text{transport}} = c_{\text{trans-var}}^{\text{source}} + c_{\text{trans-cap}}^{\text{source}} + c_{\text{trans-var}}^{\text{cwt}} + c_{\text{trans-cap}}^{\text{cwt}} + c_{\text{trans-var}}^{\text{disposal}} + c_{\text{trans-cap}}^{\text{disposal}} \quad (30)$$

$c_{\text{trans-var}}^{\text{source}}$ denotes the total variable transportation cost of acquiring freshwater, given by

$$c_{\text{trans-var}}^{\text{source}} = \sum_{s \in S} \sum_{i \in I} \sum_{m \in M} \sum_{t \in T} \frac{TS_{s,i,m} \cdot fw_{s,i,m,t}}{(1+DR)^t} \quad (31)$$

where $TS_{s,i,m}$ denotes the unit transportation cost of freshwater by transportation mode m from freshwater source s to shale site i .

The total capital investment for freshwater transportation from freshwater sources to shale sites is $c_{\text{trans-cap}}^{\text{source}}$, which is expressed as an interpolated piecewise linear cost curve, to provide an approximation of the original nonlinear function with relatively high accuracy,^{46–49} formulated as follows

$$c_{\text{trans-cap}}^{\text{source}} = \sum_{s \in S} \sum_{i \in I} \sum_{m \in M} \sum_{r \in R} FS_{s,i,m,r-1} \cdot XS_{s,i,m,r} + \sum_{s \in S} \sum_{i \in I} \sum_{m \in M} \sum_{r \in R} (tSC_{s,i,m,r} - MS_{s,i,m,r-1} \cdot XS_{s,i,m,r}) \cdot \left(\frac{FS_{s,i,m,r} - FS_{s,i,m,r-1}}{MS_{s,i,m,r} - MS_{s,i,m,r-1}} \right) \quad (32)$$

where $FS_{s,i,m,r}$ denotes the reference capital investment for transportation mode m with capacity range r from freshwater source s to shale site i .

The total variable transportation cost of wastewater between shale sites and CWT facilities, denoted as $c_{\text{trans-var}}^{\text{cwt}}$, is given by

$$c_{\text{trans-var}}^{\text{cwt}} = \sum_{i \in I} \sum_{l \in L} \sum_{c \in C} \sum_{m \in M} \sum_{t \in T} \frac{TC_{i,c,m} \cdot (wtc_{i,l,c,m,t} + wtc_{i,c,m,t})}{(1+DR)^t} \quad (33)$$

where $TC_{i,c,m}$ denotes the unit transportation cost of water by transportation mode m between shale site i and CWT facility c .

The total capital investment for wastewater transportation from shale sites to CWT facilities is $c_{\text{trans-cap}}^{\text{cwt}}$, which is also expressed as an interpolated piecewise linear cost curve, given by

$$c_{\text{trans-cap}}^{\text{cwt}} = \sum_{i \in I} \sum_{c \in C} \sum_{m \in M} \sum_{r \in R} FC_{i,c,m,r-1} \cdot XC_{i,c,m,r} + \sum_{i \in I} \sum_{c \in C} \sum_{m \in M} \sum_{r \in R} (tCC_{i,c,m,r} - MC_{i,c,m,r-1} \cdot XC_{i,c,m,r}) \cdot \left(\frac{FC_{i,c,m,r} - FC_{i,c,m,r-1}}{MC_{i,c,m,r} - MC_{i,c,m,r-1}} \right) \quad (34)$$

where $FC_{i,c,m,r}$ denotes the reference capital investment for transportation mode m with capacity range r from shale site i to CWT facility c .

$c_{\text{trans-var}}^{\text{disposal}}$ is the total variable transportation cost of wastewater from shale sites to disposal wells, given by

$$c_{\text{trans-var}}^{\text{disposal}} = \sum_{i \in I} \sum_{l \in L} \sum_{d \in D} \sum_{m \in M} \sum_{t \in T} \frac{TD_{i,d,m} \cdot wtd_{i,l,d,m,t}}{(1+DR)^t} \quad (35)$$

where $TD_{i,d,m}$ is the unit transportation cost of wastewater by transportation mode m from shale site i to disposal well d .

$c_{\text{trans-cap}}^{\text{disposal}}$ stands for the total capital investment for wastewater transportation from shale sites to disposal wells, which can be calculated by

$$c_{\text{trans-cap}}^{\text{disposal}} = \sum_{i \in I} \sum_{d \in D} \sum_{m \in M} \sum_{r \in R} FD_{i,d,m,r-1} \cdot xd_{i,d,m,r} + \sum_{i \in I} \sum_{d \in D} \sum_{m \in M} \sum_{r \in R} (tdc_{i,d,m,r} - MD_{i,d,m,r-1} \cdot xd_{i,d,m,r}) \cdot \left(\frac{FD_{i,d,m,r} - FD_{i,d,m,r-1}}{MD_{i,d,m,r} - MD_{i,d,m,r-1}} \right) \quad (36)$$

where $FD_{i,d,m,r}$ denotes the reference capital investment for transportation mode m with capacity range r from shale site i to disposal well d .

The total net present cost for handling wastewater is modeled as the sum of capital and operating costs for onsite treatment, as well as operating costs for CWT facilities, disposal wells, and onsite storage. Thus, we have the following equation

$$C_{\text{handling}} = c_{\text{onsite treatment}}^{\text{capital}} + c_{\text{onsite treatment}}^{\text{operating}} + c_{\text{cwt}} + c_{\text{disposal}} + c_{\text{storage}}^{\text{capital}} + c_{\text{storage}}^{\text{operating}} \quad (37)$$

The total capital investment for onsite treatment facilities is denoted as $c_{\text{onsite treatment}}^{\text{capital}}$, which is also expressed as an interpolated piecewise linear cost curve, formulated as follows

$$c_{\text{onsite treatment}}^{\text{capital}} = \sum_{i \in I} \sum_{o \in O} \sum_{q \in Q} FO_{i,o,q-1} \cdot y_{i,o,q} + \sum_{i \in I} \sum_{o \in O} \sum_{q \in Q} \left(\sum_{l \in L} oc_{i,l,o,q} - WO_{i,o,q-1} \cdot y_{i,o,q} \right) \cdot \left(\frac{FO_{i,o,q} - FO_{i,o,q-1}}{WO_{i,o,q} - WO_{i,o,q-1}} \right) \quad (38)$$

where $FO_{i,o,q}$ denotes the reference capital investment for level o onsite treatment with capacity range q at shale site i ; $WO_{i,o,q}$ denotes maximum capacity for level o onsite treatment facility with capacity range q at shale site i .

$c_{\text{onsite treatment}}^{\text{operating}}$ is the total operating cost for onsite treatment facilities, given by

$$c_{\text{onsite treatment}}^{\text{operating}} = \sum_{i \in I} \sum_{l \in L} \sum_{o \in O} \sum_{t \in T} \frac{VO_{i,l,o,t} \cdot wto_{i,l,o,t}}{(1+DR)^t} \quad (39)$$

where $VO_{i,l,o,t}$ is the cost of unit TDS concentration range l water treated by level o onsite treatment at shale site i at period t .

c_{cwt} denotes the total cost for CWT facilities, evaluated by

$$c_{\text{cwt}} = \sum_{i \in I} \sum_{l \in L} \sum_{c \in C} \sum_{m \in M} \sum_{t \in T} \frac{VC_{i,l,c,t} \cdot wtc_{i,l,c,m,t}}{(1+DR)^t} \quad (40)$$

where $VC_{i,l,c,t}$ is the cost of unit TDS concentration range l water treated by CWT facility c at shale site i at period t .

The total cost for disposal wells, denoted as c_{disposal} , is calculated by

$$c_{\text{disposal}} = \sum_{i \in I} \sum_{l \in L} \sum_{d \in D} \sum_{m \in M} \sum_{t \in T} \frac{VD_{i,l,d,t} \cdot wtd_{i,l,d,m,t}}{(1+DR)^t} \quad (41)$$

where $VD_{i,l,d,t}$ is the cost of unit TDS concentration range l water handled by disposal well d at shale site i at period t . $c_{\text{storage}}^{\text{capital}}$ stands for the total capital investment for onsite storage, evaluated by

$$c_{\text{storage}}^{\text{capital}} = \sum_{i \in I} CI_i \cdot sca_i \quad (42)$$

where CI_i denotes the capital investment for adding unit storage capacity at shale site i .

$c_{\text{storage}}^{\text{operating}}$ indicates the total operating cost for onsite storage, given by

$$c_{\text{storage}}^{\text{operating}} = \sum_{i \in I} \sum_{l \in L} \sum_{t \in T} \frac{CS_i \cdot wS_{i,l,t}}{(1+DR)^t} \quad (43)$$

where CS_i is the unit cost for onsite storage of water at shale site i .

The term nf denotes the net freshwater consumption. As the water treated by CWT facilities can be directly sent to surface discharge, the discharged water returns to the natural water cycle and does not count as net freshwater consumption. Thus, the net freshwater consumption is given by

$$nf = \sum_{s \in S} \sum_{i \in I} \sum_{m \in M} \sum_{t \in T} fw_{s,i,m,t} - \sum_{c \in C} \sum_{t \in T} wtcd_{c,t} \quad (44)$$

Model summary

The MILFP model (P) maximizes the profit per unit freshwater consumption, which is subject to six types of constraints: mass balance constraints, cost constraints, capacity constraints, composition constraints, lower and upper bounding constraints, and logic constraints.

The MILP model (EP) maximize the total profit of this water supply chain network, which is subject to the same constraints as in MILFP model (P), except Eqs. 27 and 44

$$(P) \quad \max \quad npf = \frac{NP - cw}{nf} \text{ given in Eq. 25}$$

s.t.

mass balance constraints (1)(2)(3)(44)

cost constraints (27)–(43)

capacity constraints (4)–(12)

composition constraint (13)

bounding constraints (14)–(20)

logic constraints (21)–(24)

$$(EP) \quad \max \quad NP - cw \text{ given in equation (26)}$$

s.t.

mass balance constraints (1)(2)(3)

cost constraints (27)–(43)

capacity constraints (4)–(12)

composition constraint (13)

bounding constraints (14)–(20)

logic constraints (21)–(24)

The optimal solution to MILP problem (EP) can be easily predicted. As this problem maximizes the total profit of this

water supply chain network, the optimal water management strategy is inclined to simply adopt the most economical options, including the primary onsite treatment and injection in disposal wells. This water management strategy neglects the freshwater consumption and the risk of overuse of disposal options. As a consequence, it deviates far from real-world cases.^{17,42} By contrast, the MILFP problem (P), the objective of which is to maximize the profit per unit freshwater consumption, leads to a balanced water management strategy. Advantages of different water management options are taken into account, and the final strategy results in a combination of different water management options. Moreover, this strategy is consistent with the real-world case. Such a comparison between problem (P) and problem (EP) clearly demonstrates the benefit of using the fractional objective function applied in this model over the linear objective. More details regarding the optimization results and comparison are presented in Case Study 1.

Solution Approaches

The proposed model (P) leads to an MILFP problem, which is a class of MINLP problem that seeks to optimize an objective function formulated as a ratio of two linear functions subject to linear constraints. Global optimization of large-scale MILFP problems can be computationally intractable due to its combinatorial nature and pseudoconvexity. In this section, we present three tailored global optimization algorithms for efficient solution of this MILFP problem, namely a parametric algorithm, a reformulation-linearization method, and a novel algorithm that integrates the Branch-and-Bound and Charnes–Cooper transformation methods.

Parametric algorithm

A parametric algorithm based on Newton's method has been recently proposed as an efficient solution approach to MILFP problems.^{50,51} This algorithm transforms the original MILFP problem to an equivalent parametric MILP problem $F(q)$ given in Figure 4, which has the same constraints as the original MILFP problem and a new objective function given as the difference between the numerator and the denominator multiplied by a parameter. The function $F(q)$ has an important property: When $F(q) = 0$, the inner MILP problem has a unique optimal solution which is exactly the same as the global optimal solution of the original MILFP problem. Based on this property, the solution of the MILFP problem involves finding the root of the equation $F(q) = 0$ as shown in the Figure 4. Although $F(q)$ does not have a closed-form analytical expression, we can apply numerical root-finding methods such as Newton's method to solve this problem. Newton's method has exact and inexact versions. The difference between these two versions is in the subproblem solution step. For the exact Newton's method applied here, we solve each parametric MILP subproblem to the global optimum, that is, 0% optimality gap. For the inexact one, we set a relative optimality gap that is less than 100% for each parametric MILP subproblem. The inexact version can potentially reduce the computational time of solving each subproblem but might need more iterations.⁵⁰ The full procedure of this parametric algorithm is shown in Figure 4.

Reformulation-linearization method

The reformulation-linearization method integrates Charnes–Cooper transformation with Glover's linearization

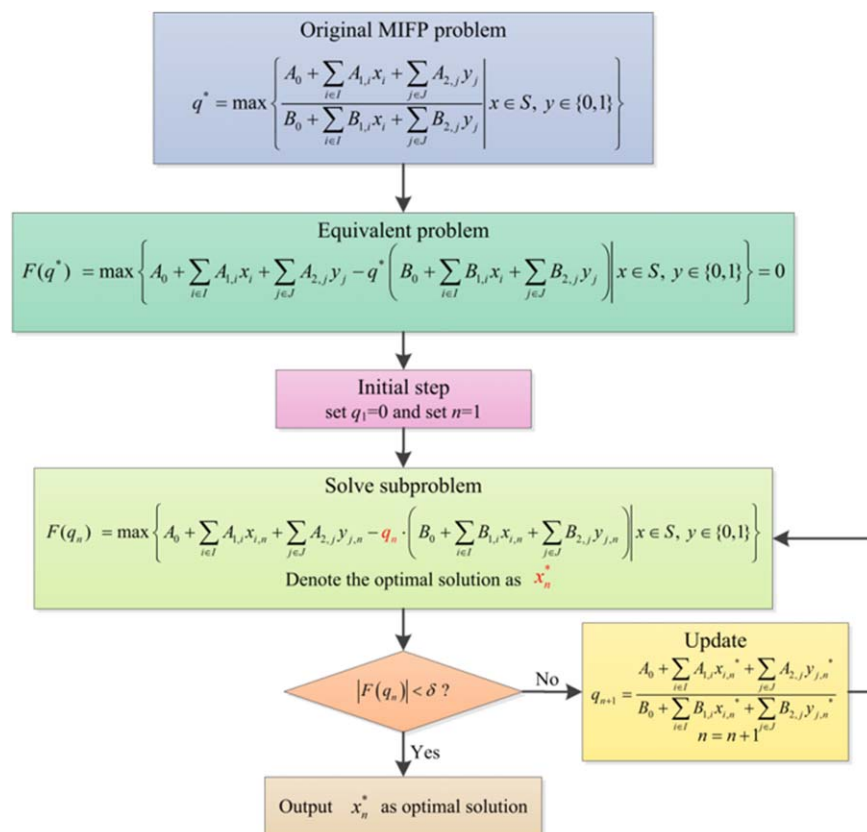


Figure 4. Flow chart of the parametric algorithm for solving MILFP problem.

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

scheme to transform the original MILFP problem to an exactly equivalent MILP problem by introducing auxiliary variables and constraints.⁵² The general equivalent relationship is given in Figure 5.

As shown above, we first apply Charnes–Cooper transformation to transform the original MILFP problem into an equivalent MINLP.⁴⁶ After that, Glover’s linearization is applied to convert the MINLP into an exactly equivalent MILP,⁴⁷ which can be solved efficiently using the branch-and-cut algorithm implemented in solvers like CPLEX.

Branch-and-Bound and Charnes–Cooper transformation method

In this section, we propose a novel MILFP solution method that combines the Branch-and-Bound algorithm and the Charnes–Cooper transformation.⁴⁶

Because MILFPs are a special class of MINLP problems, we can apply a similar Branch-and-Bound algorithm for solving MINLP problems⁵³ to the global optimization of MILFP problems. To guarantee the global optimality of the solution, the nonlinear programming (NLP) relaxation problem of each node in the Branch-and-Bound tree should be globally optimized. For MILFP problems, the NLP subproblem in each node is a linear fractional programming (LFP) problem, which can be transformed to an equivalent linear programming (LP) by applying the Charnes–Cooper transformation and then globally optimized efficiently. Thus, the integration of the Branch-and-Bound algorithm and the Charnes–Cooper transformation allows the global optimization of MILFP problems with only an LP solver.

Detailed procedures of this Branch-and-Bound and Charnes–Cooper transformation method are presented in Figure 6. It is introduced step-by-step as follows.

First, we initialize the lower and upper bounds of the MILFP problem, and store a root node in the waiting list, which is used to store all the nodes in the Branch-and-Bound tree and keeps updating as the iteration number increases. Next, we choose and remove one node from the waiting list. Generally, each node stores the information obtained from the previous iterations, including the optimal solution and the corresponding objective value, as well as the accumulated bounding constraints. Based on this information we solve the subproblem that results from relaxing the discrete conditions of the original MILFP problem.

Such a subproblem is an LFP problem. Compared to the standard Branch-and-Bound procedure that solves an NLP problem in each node, we reformulate the LFP problem into its equivalent LP problem by applying the Charnes–Cooper transformation with auxiliary variables. As shown in Figure 6, we first introduce a variable u to apply the Charnes–Cooper transformation, and then another two variables z_i and w_j are introduced to reformulate the bilinear terms resulting from this transformation. In contrast to the reformulation-linearization method, the binary variable y_j and the related constraints for the newly formulated variables w_j can be completely excluded. The discrete variables are relaxed as continuous variables in each subproblem. These constraints include

$$w_j \leq M \cdot y_j, \quad \forall j \in J \quad (45)$$

$$w_j \geq u - M \cdot (1 - y_j), \quad \forall j \in J \quad (46)$$

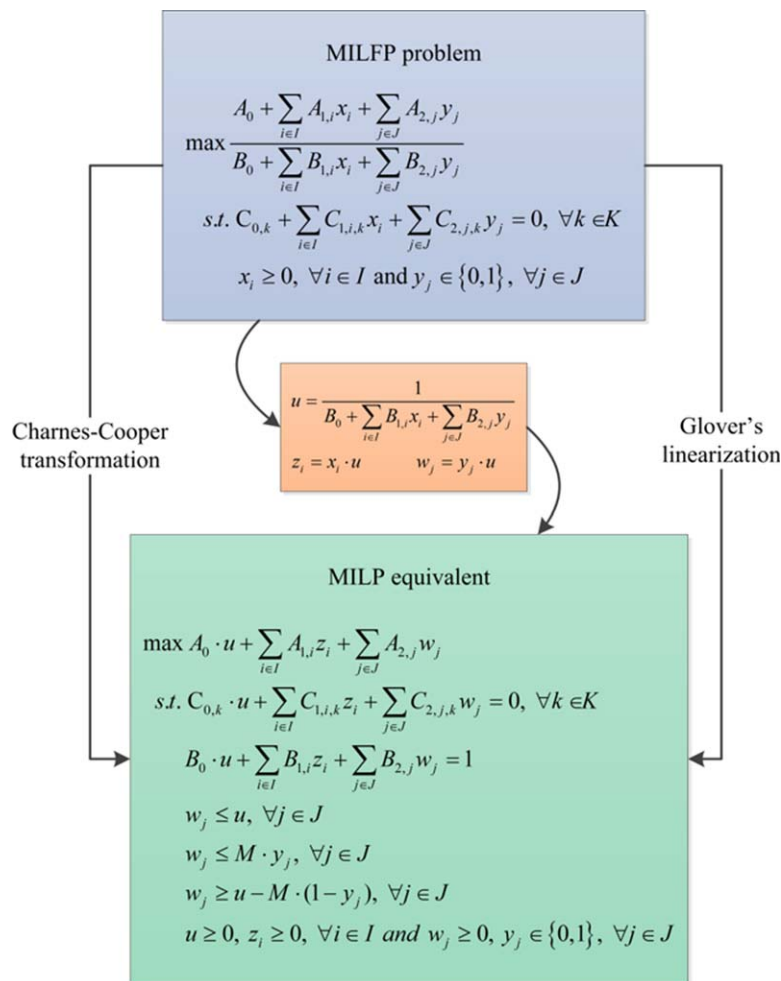


Figure 5. Flow chart of the reformulation-linearization algorithm for solving the MILFP problem.

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

For each LP subproblem, we first check its feasibility. If it is not a feasible problem, we will fathom this node directly. If this problem is feasible, we will check the integrity of its optimal solution. If the optimal solution is integral, the corresponding value will be used to update the current best solution and the lower bound of the original MINLP problem. Based on the updated lower bound, we fathom all the nodes that have objective values lower than the lower bound. If the optimal solution is nonintegral, at least one continuous variable is not integer, say y_j . We then generate two new nodes, one with additional upper bound constraint $y_j \leq \lfloor y_j \rfloor$, and the other one with additional lower bound constraint $y_j \geq \lceil y_j \rceil$. In this method, such a variable is w_j , which should be either equal to 0 or u . Thus, two new nodes are created with bound constraints $w_j \leq 0$ and $w_j \geq u$, respectively. These new nodes will be stored in the waiting list. Such a process of forming new nodes is called branching. There are different strategies of selecting the variable for branching, such as the lowest-index-first, most-fractional-integer-variable, and the use of pseudocosts strategies.^{53,54} In this work, we apply the most-fractional-integer-variable strategy.⁵⁵ It means that we select the variable which is farthest from its nearest integer value. This strategy aims at achieving the largest degradation of the objective so that more nodes can be fathomed at an early stage.

This branching and fathoming process will be repeated for each node in the waiting list. Similar to the variable

selection procedure, there are different criteria for node selection. We can select from the node with the highest bound,⁵⁶ the newest node,⁵⁷ or select the node based on estimation.⁵⁴ In this method, we choose the first criterion. By selecting the node with the highest bound currently, we expect to find the global optimal solution as soon as possible, thus, minimizing the total computational time.

The search for the optimal solution terminates when all the nodes within the waiting list are fathomed. The current best integer solution gives the global optimal solution to the original MILFP problem.

By integrating the relaxation and transformation, we are able to transform the global optimization of the original MILFP problem into the solution of a sequence of LP subproblems which can be efficiently solved by LP solvers. By branching on each “fractional value” of w_j , we can guarantee its discrete nature originated from binary variables y_j .

Summary of solution approaches

The three aforementioned MILFP algorithms all have pros and cons and might result in different computational performances when solving different MILFP problems.

For the parametric algorithm, the advantage is that we solve a sequence of MILP subproblems to obtain the global optimal solution to the original MILFP problem. Each MILP subproblem has exactly the same size as the original MILFP

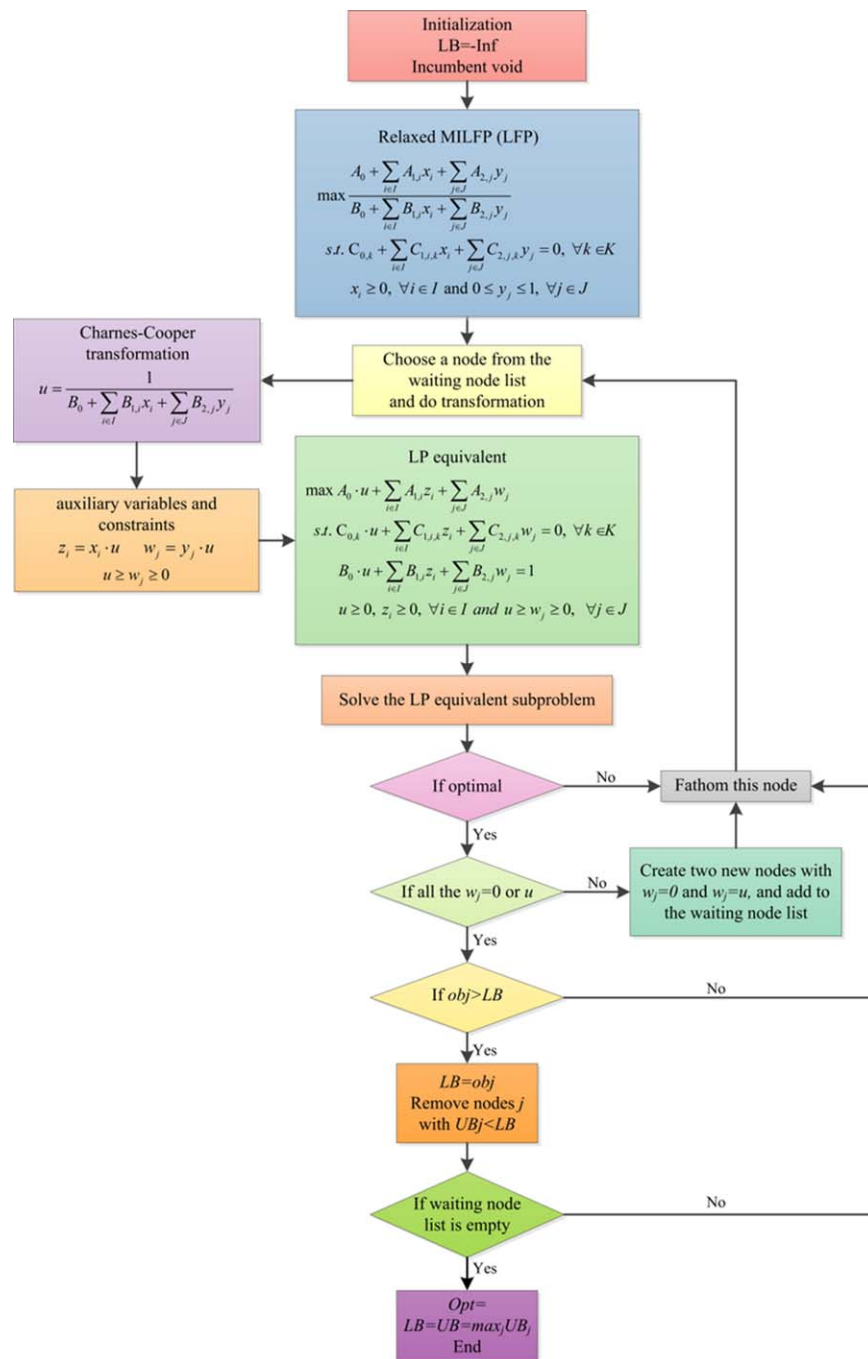


Figure 6. Flowchart of the Branch-and-Bound and Charnes–Cooper transformation method.

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

problem and can be efficiently solved by taking advantage of the efficient MILP algorithms, for example, branch-and-cut. Moreover, it has a quadratic convergence rate when using the exact Newton's method. However, the number of iterations cannot be predicted, and the optimality gap information is unavailable during the iterations.^{58–61}

The reformulation-linearization method has a clear advantage in that we only need to solve the equivalent MILP problem once to obtain the global optimal solution, and the optimality gap information is available during the solution process. However, due to the introduction of auxiliary variables and constraints, the reformulated MILP problem has a larger size than the original MILFP problem,

which might need substantially more computational time.^{62–65}

For the Branch-and-Bound and Charnes–Cooper transformation method, we solve a sequence of LP problems following the Branch-and-Bound scheme, which is much more tractable than solving a sequence of NLP subproblems. Thus, a clear strength of this algorithm is that we only need an LP solver, instead of an MILP solver required by the other two methods. However, due to the enumeration approach of the Branch-and-Bound method, the performance of this algorithm highly relies on the node selecting strategy, the tightness of the relaxation, and the number of discrete variables involved of the problem.

Table 1. Summary of Model Statistics and Computational Results for Case Study 1

	Discrete Variables	Continuous Variables	Constraints	Objective Value	Solution Time (CPUs)
MILFP problem (P)					
Parametric algorithm	297	158,213	208,080	14,970	27
Reformulation-linearization	297	158,510	208,970	14,970	294
B&B + Charnes–Cooper transformation	0 ^a	158,213	208,080	14,970	11,272
DICOPT	297	158,213	208,080	14,970	7,180
SBB	297	158,213	208,080	14,970	29,486
SCIP 3	297	158,213	208,080	N/A ^b	N/A ^b
BARON 12	297	158,213	208,080	N/A ^b	N/A ^b
MILP problem (EP)					
CPLEX 12.6	297	158,213	208,080	4,533,300	5

^aFor each iteration after reformulation and relaxation, there are no discrete variables.

^bSolver failure encountered.

Case Studies

To illustrate the application of the proposed models and solution approaches, we present two case studies based on Marcellus shale play. Detailed input data are provided in the Appendix A. Furthermore, we provide extensive computational studies to demonstrate the efficiency of proposed solution methods, details of which are included in the Appendix B. All the models and solution procedures are coded in GAMS 24.2.2⁶⁶ on a PC with Intel® Core™ i5–2400 CPU @ 3.10GHz and 8.00 GB RAM, running Window 7, 64-bit operating system. Furthermore, the MILP problems are solved using CPLEX 12.6. The MINLP solvers utilized are DICOPT and SBB as well as the global optimizers SCIP 3⁶⁷ and BARON 12.⁶⁸ The absolute optimality tolerance for all solvers is set to 0. The optimality tolerance for the outer loop in the parametric algorithm is set to 10^{-4} .

Case study 1

Case study 1 is a small-scale case study. The main goal of this case study is to demonstrate the application of the proposed models and discuss the corresponding optimization results. Through this case study we not only illustrate the practicality of the MILFP model (P) over the MILP model (EP) but also provide insights into the optimal water management strategy. As discussed in the objective function section, the objective of the MILFP problem (P) is to maximize the profit per unit freshwater consumption, and the objective of MILP problem (EP) is to maximize the total profit in the water supply chain network. In this small-scale case study, we consider a network with 2 freshwater sources, 3 shale sites, and 10 wells in each site. Freshwater withdrawal availability is estimated based on historical flowrate data with a consideration of seasonal fluctuation.^{14,69} There are three different CWT facilities and 10 available disposal wells. Wastewater is classified into three different TDS concentration ranges, ranging from 0 to 20,000 mg/L, 20,000 to 40,000 mg/L, and >40,000 mg/L, respectively, based on the TDS concentration constraints of different treatment technologies.^{26,27} We note that for Marcellus shale play, available disposal wells are mainly located far away from the shale sites in Pennsylvania (e.g., in Ohio) that are not preferable due to the high transportation cost. There are three levels of onsite treatments, that is, primary, secondary, and tertiary treatment. To be more specific, we consider the sequential treatment processes including coagulation, flocculation, and disinfection steps for the primary treatment; the application of hydrated lime ($\text{Ca}(\text{OH})_2$) and corresponding clarifier and

filter facilities for the secondary treatment; and thermal distillation technology for tertiary treatment. For the primary and secondary onsite treatment, water is partially treated, and a certain amount of make-up water is required for blending to reduce the TDS concentration to satisfy the reuse specification.^{27,41,43} For tertiary treatment, around 20% make-up water is required to reduce the TDS concentration of the flowback water below 100,000 mg/L so that it can be treated cost effectively by a desalination technology.⁷⁰ Based on the previous assumption of TDS concentration ranges, we assume that primary treatment can only handle water with TDS concentration less than 20,000 mg/L; secondary treatment is incapable of treating water with TDS concentration higher than 40,000 mg/L; and tertiary treatment is able to treat water within all the three TDS concentration ranges.⁴³ We consider pipeline and truck transportation modes for freshwater transportation from freshwater sources to shale sites. Truck is considered as the only transportation mode for wastewater from shale sites to CWT facilities and disposal wells. We also consider three capacity ranges for the pipelines used for transporting freshwater and three capacity ranges for each level of onsite treatment facilities. The planning horizon is 10 years with 520 time periods (1 week for each time period). All the input data used in this work are included in the Appendix A.

Computational Results of Case Study 1. To efficiently solve the MILFP problem (P), we applied three tailored algorithms, including a parametric algorithm based on the exact Newton's method, a reformulation-linearization method, and a novel solution algorithm that combines Branch-and-Bound and Charnes–Cooper transformation methods. We also solved the problem using general-purpose MINLP solvers, such as DICOPT and SBB, as well as the global optimizers SCIP 3 and BARON 12. To solve the MILP problem (EP), we applied the solver CPLEX 12.6. The sizes of the full-scale problems and subproblems are listed in Table 1 as well as the computational results of different solution methods for problem (P) and problem (EP).

As can be seen from Table 1, all these solution methods return the same optimal solution to the MILFP problem (P), except SCIP 3 and BARON 12. The parametric algorithm based on the exact Newton's method is the most efficient algorithm. It takes only three iterations and a total of 27 CPUs to converge to the global optimal solution. The reformulation-linearization algorithm also has excellent computational performance with a computational time of 294 CPUs. The Branch-and-Bound and Charnes–Cooper

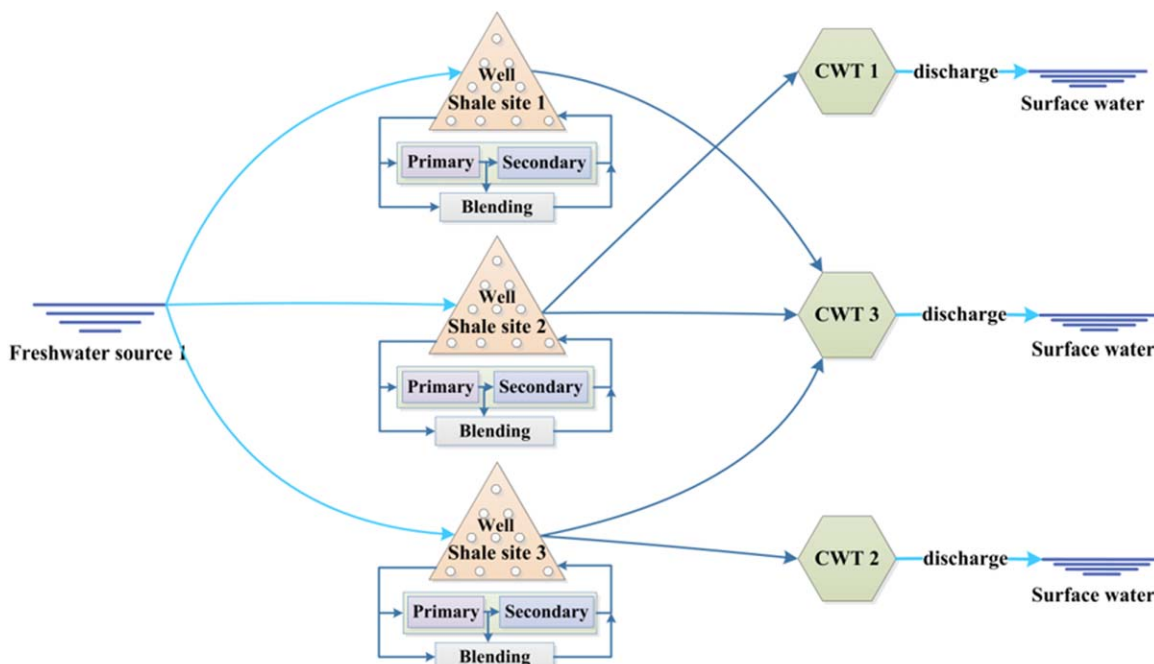


Figure 7. Water supply chain network in MILFP problem (P) in case study 1.

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

transformation algorithm returns the same objective value as the other approaches in 11,272 CPUs with a total of 183 nodes fathomed in the Branch-and-Bound tree. DICOPT is slightly more efficient than the proposed Branch-and-Bound and Charnes–Cooper transformation algorithm that it takes 7,180 CPUs to obtain the optimal solution. However, DICOPT cannot guarantee the global optimality of its solution to this MILFP problem because it is a local MINLP solver. MINLP solver SBB is also based on the Branch-and-Bound algorithm. However, it takes 29,486 CPUs to find the global optimal solution, which is much longer than that of the proposed Branch-and-Bound and Charnes–Cooper transformation algorithm. Both SCIP 3 and BARON 12 report an error and do not return any solution. In conclusion, the parametric algorithm exhibits the best computational performance among all the investigated solution methods. This computational result of this MILFP problem is consistent with those reported in the literature.^{52,59,63}

For the MILP problem (EP), the objective of which is to maximize the total profit, we directly apply the MILP solver CPLEX 12.6 to solve the problem with only five CPUs.

Optimization Results of Case Study 1. The optimal water supply chain network in MILFP problem (P) is shown in Figure 7. As there are only two freshwater sources in this small-scale case study, all the three shale sites prefer to acquire freshwater from the more economical one, which is the freshwater source 1 in this specific problem. The optimal water management strategy turns out to be a combination of CWT and onsite treatment for reuse options. All the three levels of onsite treatment are used to treat wastewater for reuse, which in turn effectively reduces the load of freshwater acquisition. As the case study is based on Marcellus shale play, where almost no disposal well is available within a short distance, underground injection option is not preferable due to the high transportation cost. The optimal objective value is \$14,970 per thousand barrels net freshwater consumption, which means that we can make about \$15 profit

for the shale gas production by consuming one barrel of freshwater.

In contrast, the water supply chain network with respect to the MILP problem (EP) is given in Figure 8. Due to the same economic reason, freshwater source 1 is chosen as the freshwater supplier for all the three shale sites. We note that in problem (EP), disposal wells are not chosen because of the same reason regarding high transportation cost. Although both CWT and onsite treatment for reuse options are used as in MILFP problem (P), the tertiary onsite treatment is not applied because of its higher treatment cost compared with CWT. It means less wastewater is treated onsite and put into reuse, and more wastewater is transported to CWTs for treatment and discharged. The recycling option from CWT is not preferred mainly due to the extra transportation cost. Based on the result of MILP problem (EP), it is easy to predict more pressure on freshwater acquisition as well as transportation in this water supply chain network. The optimal objective value of problem (EP) is \$77,358,000, indicating the total profit of shale gas production after taking the water management cost into account. The total water management cost is \$4,533,300, and for unit freshwater resource consumption, the corresponding profit is \$13,084 per thousand barrels net freshwater consumption, 14% less than that of MILFP problem (P).

This water supply chain network design and operations problem can be divided into two parts: the water supply part and the water handling part. In the following content, we give a detailed comparison between MILFP problem (P) and MILP problem (EP) with respect to these two parts.

For the water supply part, there are decisions on the selection of freshwater sources for different shale sites and the selection of transportation modes, including pipelines and trucks. As mentioned above, in both MILFP problem (P) and MILP problem (EP), freshwater source 1 is chosen as the only freshwater supplier for economic reason. Another main decision is whether to build the pipeline for freshwater

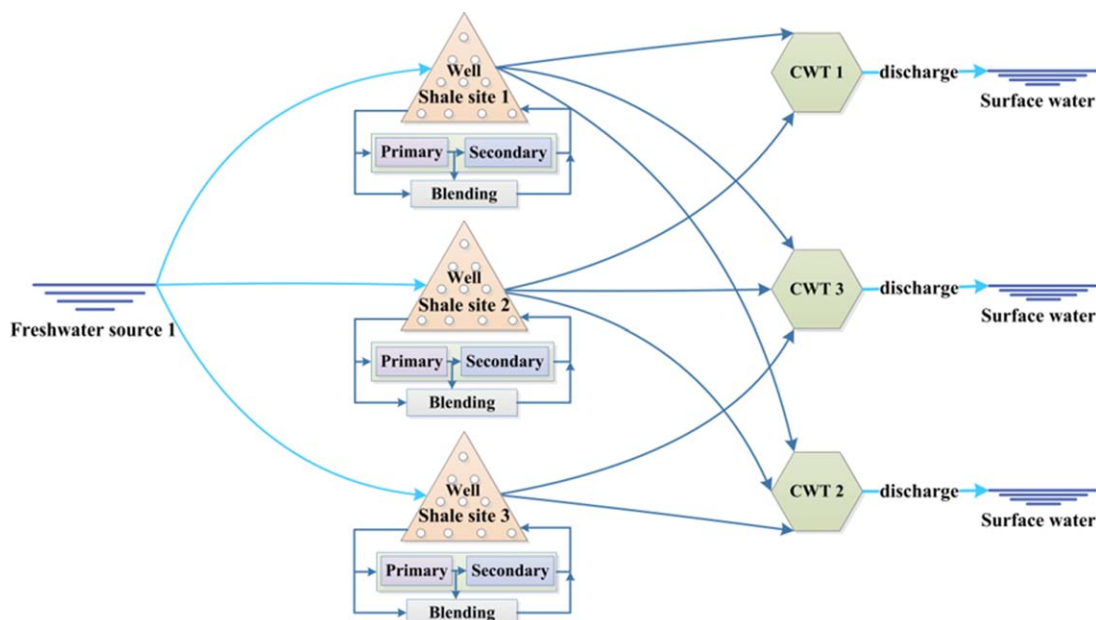


Figure 8. Water supply chain network in MILP (EP) in case study 1.

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

transportation or not. According to the optimization results, in both problems, all the freshwater is transported by pipeline. This is mainly due to its lower transportation cost in the long-term. In this case study, we consider a 10-year planning horizon, which is close to the average lifetime of shale well,^{71,72} so the high capital investment for the pipeline's construction is acceptable when distributed over such a long time period. As to the freshwater acquisition, in MILFP problem (P), a total of 5,268,306 barrels of freshwater is withdrawn from freshwater source 1 over the 10-year time horizon. The freshwater withdrawal amount of each well ranges from 169,606 to 180,039 barrels, which is close to that reported by Jiang et al.¹⁷ The corresponding total cost regarding water supply, including the freshwater acquisition and transportation cost, is \$254,473. In contrast, a total of 5,912,385 barrels of freshwater is withdrawn from freshwater source 1 in problem (EP), which is 12% more than that in problem (P). The corresponding freshwater withdrawal amount per well ranges from 196,503 to 197,747 barrels. The total water supply cost is \$281,431, 11% higher than that in problem (P). Obviously, thanks to the onsite treatment for reuse option, the freshwater consumption and the corresponding cost are significantly reduced. Detailed comparison is summarized in Table 2.

For the water handling part, the main decision is on the choice of different water management options. The detailed water management strategy is given by Figure 9, where 9(a) corresponds to the MILFP problem (P) and 9(b) is for the MILP problem (EP), respectively. As we consider a 10-year time horizon with 520 time periods, and the overall water management strategy does not change significantly with time, here we only present the optimal results from week 1 to week 12, that is, the first 3 months for the water supply chain network.

As can be observed in Figure 9, the water management strategies for both problem (P) and problem (EP) share some common features: disposal wells are not used due to the long-distance transportation cost; CWT as well as onsite treatment options are applied to treat the wastewater; the

treatment load for onsite treatment is relatively stable, while the wastewater treatment amount of CWT fluctuates with time; storage option behaves as a "buffer" to compensate the gap of wastewater treatment amount of CWT. The major difference between these two water management strategies is the preference of onsite treatment over the CWT. In the MILFP problem (P), the amount of wastewater treated onsite and reused is almost twice as much as that in MILP problem (EP). As a result, less wastewater is transported to CWT facilities for treatment, and the inventory level is lower as well in the MILFP problem (P). We note that though the recycling option of treated water from CWT to shale site is considered in this model, this option is not chosen due to the extra transportation cost for this recycling path. Consequently, less water is reused onsite or recycled from CWT facilities, and more freshwater is required at each time period in the MILP problem (EP).

A summary of the optimal water management options for water with different TDS concentration ranges is given by Figure 10, where 10a corresponds to the MILFP problem (P) and 10b stands for the MILP problem (EP). We can see that in both (P) and (EP) problems, the range 1 water, which has relatively lower TDS concentration (0–20,000 mg/L) in this model, tends to be treated by primary onsite treatment. Similarly, the range 2 water, which has a medium TDS concentration (20,000–40,000 mg/L), is treated by the secondary

Table 2. Results Comparison Regarding Water Supply Part Between MILFP Problem (P) and MILP Problem (EP)

	MILFP Problem (P)	MILP Problem (EP)	Difference
Total freshwater withdrawal (bbl)	5,268,306	5,912,388	+12%
Average freshwater withdrawal per well (bbl/well)	175,610	197,080	+12%
Total water supply cost (\$)	254,473	281,431	+11%

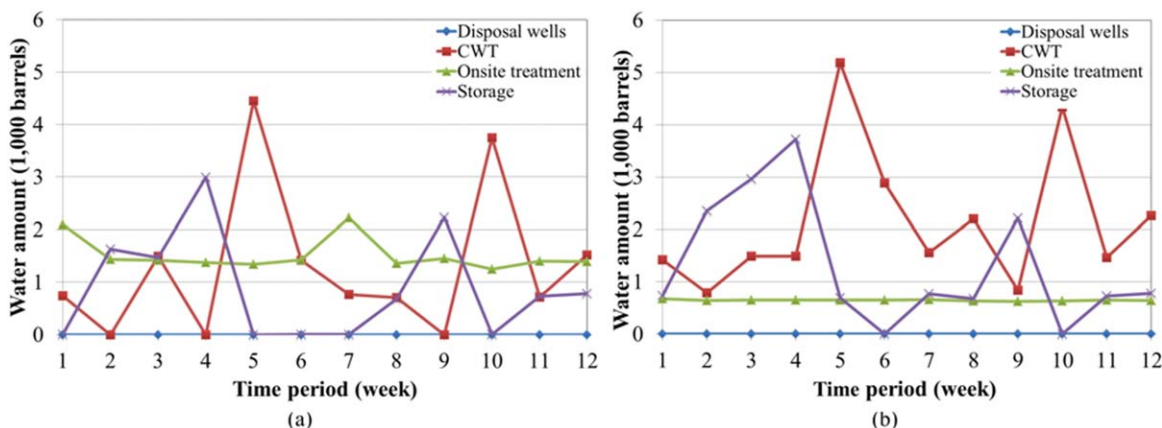


Figure 9. Optimal water management strategy for (a) MILFP problem (P) and (b) MILP problem (EP) in case study 1.

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

onsite treatment. The remaining range 3 wastewater with TDS concentration higher than 40,000 mg/L is treated by CWT facilities or tertiary onsite treatment. In MILFP problem (P), as our objective is to maximize the profit per unit freshwater consumption, and onsite treatment option can reduce the transportation cost and freshwater consumption simultaneously by treating wastewater onsite and blending it with freshwater for reuse, the onsite treatment is preferred than the CWT option. The latter one cannot reduce the freshwater consumption cost effectively because of the extra transportation cost. Meanwhile, in MILP problem (EP), the objective is to maximize the total profit with respect to water management, and CWT is a more economic option compared with tertiary onsite treatment. The technology considered for tertiary onsite treatment in this model is thermal distillation technology, which is highly energy intensive and suffers from high operating cost. The different objectives as well as the unique features of CWT and onsite treatment options lead to different water management strategies. About 69% of the range 3 water is treated by tertiary onsite treatment, and the remaining 31% is transported to CWT for treatment and discharge in MILFP problem (P). However, in MILP problem (EP), all the range 3 water is sent to CWT for treatment and discharge.

The overall cost distribution of different water management sections is given by Figure 11, where 11a corresponds to the MILFP problem (P) and 11b stands for the MILP

problem (EP). The total water management cost in MILFP problem (P) is \$5,346,139, 18% greater than that in MILP problem (EP), which is \$4,533,300. However as mentioned above, the profit gained corresponding to unit freshwater consumption is \$14,970 per thousand barrels of freshwater consumption in problem (P), 14% greater than \$13,084 per thousand barrels of freshwater consumption in problem (EP), which indicates a higher freshwater utilization efficiency. As to the detailed breakdown of total water management cost, the CWT facilities contribute to 11% of the overall cost for water management in MILFP problem (P), while in (EP), this number is 51%; onsite treatment accounts for 79% of the total cost in problem (P), including capital investment and operating cost, while in problem (EP) only 13% of the total cost comes from onsite treatment. Due to the extensive application of onsite treatment and reuse in MILFP problem (P), the stress on freshwater withdrawal, related transportation among freshwater sources, shale sites, and CWT facilities, and onsite storage are relieved. As a result, the freshwater acquisition cost, storage cost, and transportation cost are all lower than those in MILP problem (EP), especially the transportation cost that decreases from 29% to only 6% of the total water management cost.

Based on the comparison above, we conclude that it is impossible to obtain a good balance between cost effectiveness and freshwater conservancy by simply minimizing the total cost. In the MILP problem (EP), most of the

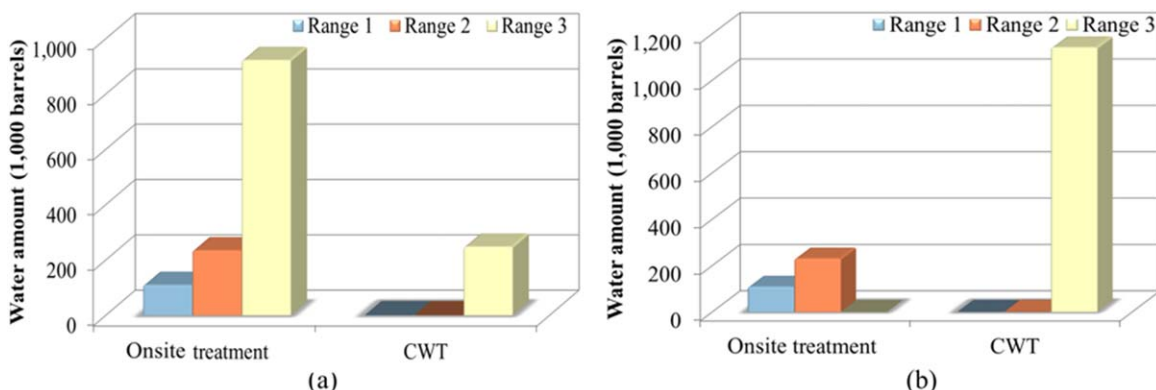


Figure 10. Optimal water management options for the three TDS concentration ranges for (a) MILFP problem (P) and (b) MILP problem (EP) in case study 1.

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

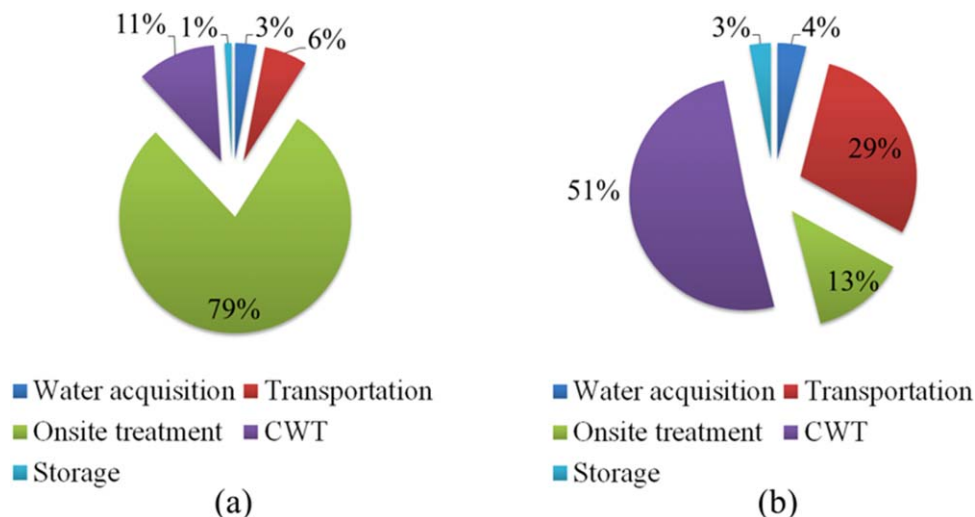


Figure 11. Cost breakdown of water management options in (a) MILFP problem (P) and (b) MILP problem (EP) of case study 1.

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

wastewater is transported to the CWT for treatment and direct discharge. By comparison, the fractional objective function in problem (P) gives a more efficient and practical water management strategy, through which a more stable water management strategy is obtained with more water reuse, less freshwater consumption, and less stress on transportation as well as storage. Such a water management strategy is also close to the real one applied at Marcellus shale play.⁴²

Case study 2

We further consider a large-scale case study on the design and operations of the water supply chain network based on Marcellus shale play. As the MILFP model (P) has been proven to be more suitable for this problem than the MILP model (EP), all the results presented in this section are based on MILFP problem (P). The main goal is to further compare computational performances of different algorithms in solving large-scale MILFP problem, and to give some meaningful quantitative results regarding the water management problem in Marcellus shale gas production.

In case study 2, we consider 10 freshwater sources, 10 shale sites, and 10 wells at each shale site. There are five CWT facilities and 50 disposal wells. The remaining input data of case study 2 are almost the same as in case study 1,

including the water composition, levels of onsite treatment and corresponding technologies, capacity ranges regarding transportation modes and onsite treatment facilities, and the planning horizon. Similarly, major input data are included in the appendix.

The resulting problem in case study 2 is a large-scale MILFP problem, which has 2,340 binary variables, 1,945,171 continuous variables, and 2,618,391 constraints.

Computational Results of Case Study 2. We apply the same solution strategies as in case study 1 and the corresponding problem sizes and computational results are listed in Table 3.

As can be seen in Table 3, the parametric algorithm successfully returns the optimal solution within only 499 CPUs. Even though the performance of reformulation-linearization method is comparable to the parametric algorithm in case study 1, as the problem scales up in case study 2, it takes 21,158 CPUs to find the optimal solution, which is much longer than 499 CPUs. Similarly, due to the heavy burden of doing branching for each discrete variable, the Branch-and-Bound and Charnes–Cooper transformation method fails to find a feasible solution in this large-scale problem, but an upper bound of 14,802 is given, which behaves as a good estimation of the global optimal solution. General-purpose solvers perform worse than the tailored MILFP algorithms

Table 3. Summary of Model Statistics and Computational Results for Case Study 2

	Discrete Variables	Continuous Variables	Constraints	Objective Value	Solution Time (CPUs)
Parametric algorithm	2,340	1,945,171	2,618,391	14,797	499
Reformulation-linearization	3,990	1,949,162	2,630,362	14,797	21,158
B&B + Charnes–Cooper transformation	0 ^a	1,945,171	2,618,391	-Inf-14,802 ^b	36,000
DICOPT	2,340	1,945,171	2,618,391	N/A ^c	36,000
SBB	2,340	1,945,171	2,618,391	N/A ^c	36,000
SCIP 3	2,340	1,945,171	2,618,391	N/A ^d	N/A ^d
BARON 12	2,340	1,945,171	2,618,391	N/A ^d	N/A ^d

^aFor each iteration after reformulation and relaxation, there are no discrete variables left.

^bOnly lower and upper bounds returned within 36,000 s (10 h).

^cExceeded specified time limit of 36,000 s (10 h) with no feasible solution returned.

^dSolver failure encountered.

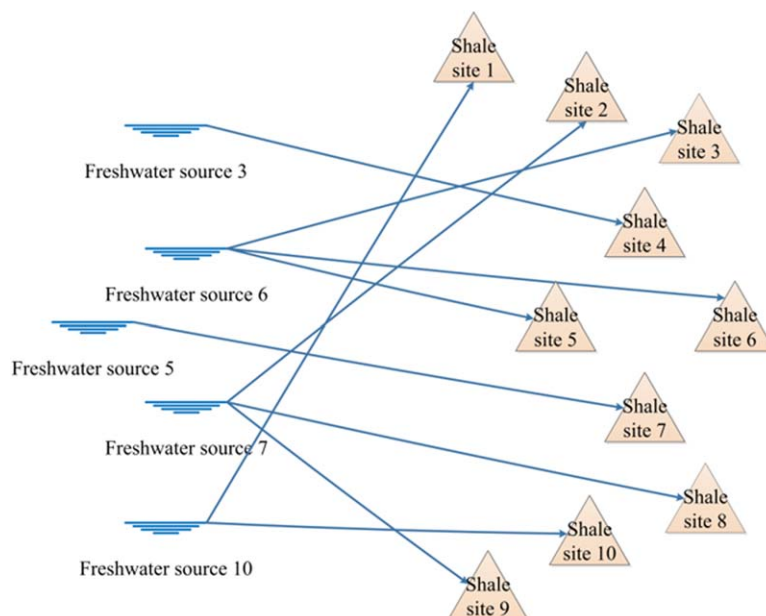


Figure 12. Optimal pipeline construction network of case study 2.

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

mentioned above. Both DICOPT and SBB fail to find a feasible solution within the 36,000 CPUs time limit. Global optimizers SCIP 3 and BARON 12 encounter the same solver failure issues as in case study 1.

Thus, the parametric algorithm is still the most efficient solution approach for this MILFP problem compared with other solution methods. It maintains excellent computational performance in solving this large-scale MILFP problem and takes only three iterations to converge to the optimal solution. The reformulation-linearization method though performs well in solving the small-scale MILFP problem in case study 1, its computational efficiency drops significantly

from 294 CPUs to 21,158 CPUs as the problem scales up. The Branch-and-Bound and Charnes–Cooper transformation method transforms the original, complicated MILFP problem into a sequence of LP subproblems which is theoretically much easier to solve. However, in practice it does not significantly reduce the computational time in each node in the Branch-and-Bound tree. Furthermore, as the problem size increases, the number of nodes might increase exponentially, and the overall computational performance of this method is significantly affected. As a consequence, the algorithm that combines Branch-and-Bound and Charnes–Cooper transformation methods does not perform efficiently in solving the

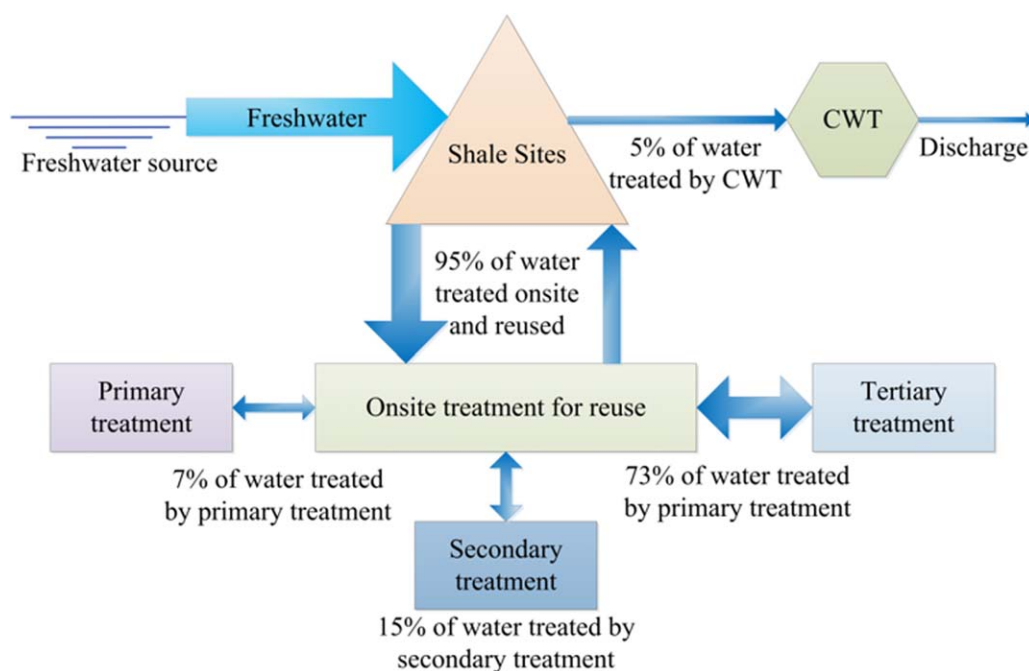


Figure 13. Optimal water management strategy in case study 2.

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

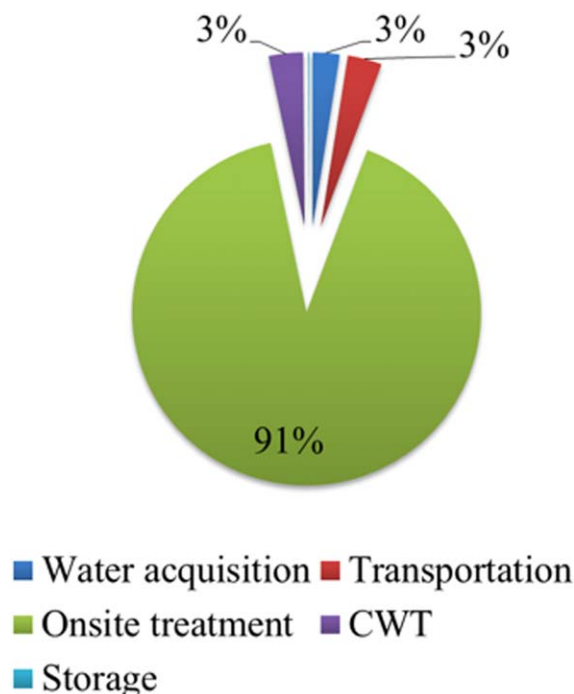


Figure 14. Cost breakdown of water management options of case study 2.

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

large-scale MILFP problem. However, some useful information such as the upper bound can be obtained in the solution. General-purpose MINLP solvers, DICOPT and SBB are also not efficient compared with the three tailored MILFP solution methods. They both fail to return any feasible solution within the time limit. Global optimizers SCIP 3 and BARON 12 have a high chance to encounter solver failures for large-scale problems.

Optimization Results of Case Study 2. In this section, we present the optimization results obtained by the parametric algorithm, as it is the only solution approach that gives the optimal solution within the computational time limit.

The optimal objective value is \$14,797 per thousand barrels of freshwater consumption, which is very close to \$14,970 per thousand barrels of freshwater consumption obtained in case study 1. This result is reasonable, because by changing the problem size only, there should be no significant difference between the unit profits with almost identical input data. A total of 17,792,000 barrels of freshwater is transported from freshwater sources to shale sites, and the gross freshwater consumption per shale well is about 177,920 barrels. As all the freshwater is transported by pipeline, we only present the optimal pipeline network in Figure 12. As can be seen, the complexity of this network increases significantly in this large-scale case study. Moreover, we identify freshwater sources 6 and 7 as attractive freshwater sources, which supply multiple shale sites with freshwater. This result is similar to that in the case study 1, indicating that using pipeline to transport freshwater is more economical than using trucks from a long-term perspective in shale gas production.

The optimal water management strategy is summarized in Figure 13. As there are much more shale sites and specific

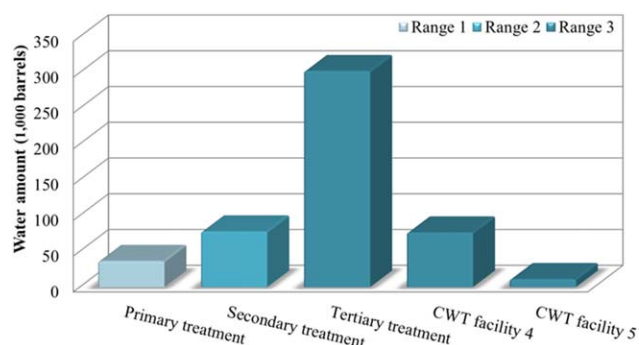


Figure 15. Optimal water management strategy for the three TDS concentration ranges in shale site 5 in case study 2.

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

water management options than that in case study 1, we only present an overview of the optimal water management strategy here. As we can see, the optimal water management strategy in case study 2 is similar to that in case study 1. Disposal wells are still not used due to high transportation cost. A total of 363,788 barrels of range 1 water is treated by primary onsite treatment, and 780,315 barrels of range 2 water is treated by secondary onsite treatment. All of remaining 3,903,484 barrels of range 3 water is either treated onsite by tertiary treatment, which accounts for 73% of the total amount, or transported to CWT for treatment and discharge, accounting for 5% of the total wastewater.

The distribution of water management costs is shown in Figure 14. A total of \$18,911,480 cost is obtained, where onsite treatment accounts for 91% of the total cost, including capital investment as well as operating cost. CWT contributes 3% of the total cost, and transportation cost is 3% of the total. The remaining 3% cost includes the costs for water acquisition and storage.

To present the detailed water management strategy for a certain shale site, we select one shale site, indexed as shale site 5, among the ten shale sites and present the corresponding optimization result.

According to the optimization result, in the 10-year time horizon, shale site 5 withdraws 1,836,480 barrels of freshwater from freshwater source 6 through pipeline, and the transportation capacity of pipeline is chosen as 4,069 barrels per week.

Figure 15 illustrates the optimal strategy for handling different TDS concentration ranges wastewater in shale site 5. We note that all 36,313 barrels of range 1 water is treated by primary onsite treatment for reuse, and 77,698 barrels of range 2 water is treated by secondary onsite treatment. 302,024 barrels of range 3 water is treated by tertiary onsite treatment for reuse, and the remaining 87,373 barrels range 3 water is transported to CWT facilities 4 and 5 for treatment and discharge. In total, about 83% of wastewater is treated onsite and reused, while 17% are treated by CWT and discharged. This specific water management strategy for shale site 5 is consistent with the overall strategy.

Conclusion

In this article, we presented a novel optimization model for the optimal design and operations of water supply chain

networks for shale gas production. The objective function was given as the profit per unit freshwater consumption. The main goal was to reduce the total cost of a water supply chain network for shale gas production while reducing the net freshwater consumption. Such a problem was formulated as an MILFP problem. To demonstrate the practicality of the fractional objective function of the MILFP model, we further introduced an MILP model for comparison. The objective of the MILP model was to maximize the total profit of a water supply chain network subject to the same constraints of the MILFP model. While the models were general enough to consider multiple water management options, we focused on the disposal, CWT, and onsite treatment options in this work. Furthermore, three levels of onsite treatment were considered, namely primary, secondary, and tertiary treatment. Primary treatment involved simple filtration and removal of FOG. Secondary treatment included lime softening and clarification. Tertiary treatment involved thermal distillation for desalination to reduce the TDS concentration. Two water transportation modes as pipeline and truck were taken into account. To solve this complex MILFP problem, two tailored algorithms adopted from literature were applied, including a parametric algorithm and a reformulation-linearization method. In addition, we proposed a novel solution algorithm that combines Branch-and-Bound and Charnes–Cooper transformation methods. Thus, the global optimal solution for the original MILFP problem can be obtained by solving a sequence of LP subproblems corresponding to the nodes in the Branch-and-Bound tree.

To illustrate the proposed models and solution methods, two case studies on the long-term design and operations of water supply chain networks for shale gas production were presented based on Marcellus shale play. In the small-scale case study, the optimal water management strategies obtained from MILFP problem (P) and MILP problem (EP) were carefully analyzed and discussed. The superiority of MILFP problem (P) over MILP problem (EP) was validated. Moreover, the onsite treatment option turned out to be appealing in improving freshwater conservancy, maintaining a stable water flow, and reducing transportation burden. In the large-scale case study based on Marcellus shale play, the maximum profit obtained by consuming unit freshwater was \$14,797 per thousand barrels freshwater. The computational results indicated the outstanding efficiency of the parametric algorithm in solving large-scale MILFP problems. Compared with general-purpose MINLP solvers, such as SBB and DICOPT, as well as global optimizers SCIP 3 and BARON 12, the parametric algorithm could reduce the computational time by one or even three orders of magnitude. The reformulation-linearization method had comparable computational performance to the parametric algorithm when solving the smaller MILFP problem. However, it failed to solve the large-scale problem within a 10-hour computational time limit. The Branch-and-Bound and Charnes–Cooper transformation algorithm did not show efficient computational performance mainly due to the enumerative nature of the Branch-and-Bound method. However, it showed its advantage over other general MINLP solvers such as DICOPT and SBB. The parametric algorithm maintained its computational efficiency in both small-scale and large-scale case studies and out-performed all the other MILFP solution methods.

In this work, as the main focus is on water management in shale gas production, we solely consider a separated water supply chain by assuming all the input from the shale gas supply chain as known parameters. However, due to the close connection between the shale gas and water systems, we realize the realistic meaning of combining these two networks together. In the next step, we may consider a comprehensive model integrating both the shale gas supply and water supply chain to provide a more meaningful guidance for shale gas industry.

Acknowledgment

We gratefully acknowledge the financial support from the Institute for Sustainability and Energy at Northwestern University (ISEN).

Notation

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
 J = set of wells indexed by j
 L = set of TDS concentration ranges indexed by l ($l1$: 0–20,000 mg/L; $l2$: 20,000–40,000 mg/L; $l3$: 40,000–Inf mg/L)
 M = set of transportation modes indexed by m ($m1$: truck; $m2$: pipeline)
 O = set of different levels of onsite treatments indexed by o ($o1$: primary treatment; $o2$: secondary treatment; $o3$: tertiary treatment)
 Q = set of capacity ranges for onsite treatments indexed by q
 R = set of capacity ranges for transportation modes indexed by r
 S = set of freshwater resources indexed by s
 T = set of time periods indexed by t

Subset

$O(l)$ = subset of set O for onsite treatment that are capable of treating TDS concentration range l water

Parameters

$CC_{i,j,t}$ = correlation coefficient for shale gas production and production of produced water from well j at shale site i at time period t
 CS_i = variable cost for the storage of unit water at shale site i
 CI_i = capital investment for adding unit storage capacity at shale site i
 DR = discount rate per time period in calculating net present value
 $FC_{i,c,m,r}$ = reference capital investment for transportation mode m with range r from shale site i to CWT facility c
 $FD_{i,d,m,r}$ = reference capital investment for transportation mode m with range r from shale site i to disposal well d
 $FO_{i,o,q}$ = reference capital investment for level o onsite treatment with capacity range q at shale site i
 $FR_{s,t}$ = available amount of freshwater for source s at time period t
 $FS_{s,i,m,r}$ = reference capital investment for transportation mode m with range r from source s to shale site i
 LC_l = recovery factor for the CWT treatment method treating TDS concentration range l water
 $LO_{l,o}$ = recovery factor for level o onsite treatment technologies treating TDS concentration range l water
 $MC_{i,c,m,r}$ = maximum capacity of range r transportation mode m from shale site i to CWT facility c
 $MD_{i,d,m,r}$ = maximum capacity of range r transportation mode m from shale site i to disposal well d
 $MS_{s,i,m,r}$ = maximum capacity of range r transportation mode m from source s to shale site i
 RF_o = ratio of freshwater to wastewater required for blending for level o onsite treatment
 $RW_{i,j,t}$ = amount of water required for hydraulic fracturing for well j at shale site i at time period t
 SC_i = initial storage capacity at shale site i
 SM_i = maximum additional storage capacity can be installed at shale site i
 $SP_{i,t}$ = average revenue per unit shale gas production for shale site i at time period t

$TC_{i,c,m}$ = variable transportation costs per unit water between shale site i and CWT facility c by transportation mode m
 $TD_{i,d,m}$ = variable transportation costs per unit water between shale site i and disposal well d by transportation mode m
 $TS_{s,i,m}$ = variable transportation costs per unit water between source s and shale site i by transportation mode m
 $VC_{i,l,c,t}$ = cost of unit TDS concentration range l water treated by CWT facility c at shale site i at time period t
 $VD_{i,l,d,t}$ = cost of unit TDS concentration range l water treated by disposal well d at shale site i at time period t
 $VO_{i,o,t}$ = cost of unit TDS concentration range l water treated by level o onsite treatment at shale site i at time period t
 WA_s = unit freshwater acquirement costs from source s
 $WC_{c,t}$ = capacity of CWT facility c to water at time period t
 $WD_{d,t}$ = capacity of disposal well d to handle wastewater at time period t
 $WO_{i,o,q}$ = maximum capacity of level o onsite treatment facility with capacity range q at shale site i
 $WP_{i,j,l,t}$ = production of TDS concentration range l water from well j at shale site i at time period t

Continuous variables

$fw_{s,i,m,t}$ = amount of freshwater acquired from source s for well j at shale site i using transportation mode m at time period t
 $oc_{i,l,o,q}$ = treatment capacity for TDS concentration range l water treated by level o onsite treatment with capacity range q at shale site i
 sca_i = additional storage capacity installed at shale site i
 $tcc_{i,c,m,r}$ = transportation capacity for range r transportation mode m from shale site i to CWT facility c
 $tdc_{i,d,m,r}$ = transportation capacity for range r transportation mode m from shale site i to disposal well d
 $tsc_{s,i,m,r}$ = transportation capacity for range r transportation mode m from source s to shale site i
 $ws_{i,l,t}$ = amount of TDS concentration range l produced water being stored at shale site i at time period t
 $wtc_{i,l,c,m,t}$ = amount of TDS concentration range l produced water transported with transportation mode m and treated with CWT facility c at shale site i at time period t
 $wtd_{c,t}$ = amount of treated water at CWT facility c disposed directly to surface water at time period t
 $wtr_{i,c,m,t}$ = amount of treated water at CWT facility c recycled to shale site i with transportation mode m at time period t
 $wtd_{i,l,d,m,t}$ = amount of TDS concentration range l produced water transported with transportation mode m and handled by disposal well d at shale site i at time period t
 $wto_{i,l,o,t}$ = amount of TDS concentration range l produced water treated level o onsite treatment at shale site i at time period t

Binary variables

$xc_{i,c,m,r}$ = 0–1 variable. Equal to 1 if capacity range r transportation mode m is installed to transport water from shale site i to CWT facility c
 $xd_{i,d,m,r}$ = 0–1 variable. Equal to 1 if capacity range r transportation mode m is installed to transport water from shale site i to disposal well d
 $xs_{s,i,m,r}$ = 0–1 variable. Equal to 1 if capacity range r transportation mode m is installed to transport freshwater from source s to shale site i
 $y_{i,o,q}$ = 0–1 variable. Equal to 1 if level o onsite treatment facility with capacity range q is installed on shale site i

Literature Cited

- EIA. Review of Emerging Resources: U.S. Shale Gas and Shale Oil Plays. Washington, DC: U. S. Energy Information Administration, 2011.
- EIA. World Shale Gas Resources: An Initial Assessment of 14 Regions Outside the United States. U. S. Energy Information Administration, 2011.
- Hughes JD. *Drill, Baby, Drill: Can Unconventional Fuels Usher in a New Era of Energy Abundance?* 2013.
- EIA. Annual Energy Outlook 2013. Washington, DC: U. S. Energy Information Administration, 2013.
- Wang Q, Chen X, Jha AN, Rogers H. Natural gas from shale formation—the evolution, evidences and challenges of shale gas

- revolution in United States. *Renew Sust Energy Rev.* 2014;30: 1–28.
- Gregory KB, Vidic RD, Dzombak DA. Water management challenges associated with the production of shale gas by hydraulic fracturing. *Elements.* 2011;7:181–186.
- Vengosh A, Warner N, Jackson R, Darrah T. The effects of shale gas exploration and hydraulic fracturing on the quality of water resources in the United States. In: *Proceedings of the Fourteenth International Symposium on Water-Rock Interaction, Wri 14*, vol. 7. 2013:863–866.
- Hughes JD. A reality check on the shale revolution. *Nature.* 2013; 494:307–308.
- Ehlinger VM, Gabriel KJ, Noureldin MMB, El-Halwagi MM. Process design and integration of shale gas to methanol. *ACS Sustain Chem Eng.* 2013;2:30–37.
- Nicot J-P, Scanlon BR. Water use for shale-gas production in Texas, U.S. *Environ Sci Technol.* 2012;46:3580–3586.
- He C, You F. Shale gas processing integrated with ethylene production: novel process designs, exergy analysis, and techno-economic analysis. *Ind Eng Chem Res.* 2014;53:11442–11459.
- Mauter MS, Palmer VR, Tang Y, Behrer AP. The next frontier in United States shale gas and tight oil extraction: strategic reduction of environmental impacts. *Belfer center for science and international affairs discussion paper series.* 2013.
- Small MJ, Stern PC, Bomberg E, Christopherson SM, Goldstein BD, Israel AL, Jackson RB, Krupnick A, Mauter MS, Nash J, North DW, Olmstead SM, Prakash A, Rabe B, Richardson N, Tierney S, Webler T, Wong-Parodi G, Zielinska B. Risks and risk governance in unconventional shale gas development. *Environ Sci Technol.* 2014;48: 8289–8297.
- Yang L, Manno J, Grossmann IE. Optimization models for shale gas water management. *AIChE J.* 2014;60:3490–3501.
- Mauter M, Palmer V. Expert elicitation of trends in marcellus oil and gas wastewater management. *J Environ Eng.* 2014;140: B4014004.
- Mauter MS, Alvarez PJJ, Burton A, Cafaro DC, Chen W, Gregory KB, Jiang G, Li Q, Pittock J, Reible D, Schnoor JL. Regional variation in water-related impacts of shale gas development and implications for emerging international plays. *Environ Sci Technol.* 2014; 48:8298–8306.
- Jiang M, Hendrickson CT, VanBriesen JM. Life cycle water consumption and wastewater generation impacts of a marcellus shale gas well. *Environ Sci Technol.* 2013;48:1911–1920.
- EPA. Plan to Study the Potential Impacts of Hydraulic Fracturing on Drinking Water Resources. Washington, DC: Office of Research and Development U.S. Environmental Protection Agency, 2011.
- API. Water management associated with hydraulic fracturing. In: API, 1st ed. Washington, DC: American Petroleum Institute, 2010.
- Paper W. *US Shale Gas—Anunconventional Resource, Unconventional Challenge.* Halliburton, 2008.
- Nicot JP, Scanlon BR, Reedy RC, Costley RA. Source and fate of hydraulic fracturing water in the barnett shale: a historical perspective. *Environ Sci Technol.* 2014;48:2464–2471.
- Soeder DJ, Kappel WM. Water Resources and Natural Gas Production from the Marcellus Shale. Virginia: US Department of the Interior, US Geological Survey Reston, 2009.
- Rahm BG, Riha SJ. Toward strategic management of shale gas development: regional, collective impacts on water resources. *Environ Sci Policy.* 2012;17:12–23.
- Karapataki C. *Techno-Economic Analysis of Water Management Options for Unconventional Natural Gas Developments in the Marcellus Shale* [Master thesis]. Cambridge, MA: Engineering Systems Division, Technology and Policy Program, Massachusetts Institute of Technology, 2012.
- Slutz JA, Anderson JA, Broderick R, Horner PH. Key shale gas water management strategies: an economic assessment. In: *Paper presented at International Conference on Health Safety and Environment in Oil and Gas Exploration and Production*, 2012.
- Gaudlip AW, Paugh LO. Marcellus shale water management challenges in Pennsylvania. In: *Shale Gas Production Conference.* Fort Worth, TX, 2008.
- Veil JA. *Final Report Water Management Technologies Used by Marcellus Shale Gas Producers.* Argonne, IL: U.S. Department of Energy, July 2010.

28. Cafaro DC, Grossmann IE. Strategic planning, design, and development of the shale gas supply chain network. *Aiche J.* 2014;60: 2122–2142.
29. Centner TJ, O'Connell LK. Unfinished business in the regulation of shale gas production in the United States. *Sci Total Environ.* 2014; 476–477:359–367.
30. Mallapragada DS, Duan G, Agrawal R. From shale gas to renewable energy based transportation solutions. *Energy Policy.* 2014;67:499–507.
31. Rich A, Grover JP, Sattler ML. An exploratory study of air emissions associated with shale gas development and production in the Barnett Shale. *J Air Waste Manage Assoc.* 2014;64:61–72.
32. McGowan F. Regulating innovation: European responses to shale gas development. *Environ Politics.* 2014;23:41–58.
33. Meng QM. Modeling and prediction of natural gas fracking pad landscapes in the Marcellus Shale region, USA. *Landsc Urban Plan.* 2014;121:109–116.
34. McHugh T, Molofsky L, Daus A, Connor J. Comment on “an evaluation of water quality in private drinking water wells near natural gas extraction sites in the barnett shale formation”. *Environ Sci Technol.* 2014;48:3595–3596.
35. Goldstein BD. The importance of public health agency independence: Marcellus shale gas drilling in Pennsylvania. *Am J Public Health.* 2014;104:e13–e15.
36. Vidic RD, Brantley SL, Vandenbossche JM, Yoxtheimer D, Abad JD. Impact of shale gas development on regional water quality. *Science.* 2013;340:1235009.
37. Horner P, Halldorson B, Slutz JA. Shale gas water treatment value chain—a review of technologies including case studies. In: *Paper presented at SPE Annual Technical Conference and Exhibition*, 2011.
38. DOE. The Water-Energy Nexus: Challenges and Opportunities. U.S. Department Of Energy, 2014.
39. Puder MG, Veil JA. *Offsite Commercial Disposal of Oil and Gas Exploration and Production Waste: Availability, Options, and Costs.* Argonne National Laboratory for the U.S. Department of Energy, Office of Fossil Energy, National Energy Technology Laboratory, 2006.
40. Seydor SM, Clements E, Pantelemonitis S, Deshpande V. *Understanding the Marcellus Shale Supply Chain.* University of Pittsburgh, Katz Graduate School of Business, 2012.
41. David A. Considerations for treating water associated with shale gas development. In: *Water/Energy Sustainability Symposium 2010 Annual Forum.* Pittsburgh, Pennsylvania, 2010.
42. Wilson JM, VanBriesen JM. Oil and gas produced water management and surface drinking water sources in Pennsylvania. *Environ Pract.* 2012;14:288–300.
43. Acharya HR, Henderson C, Matis H, Kommepalli H, Wang H. Cost Effective Recovery of Low TDS Frac Flowback Water for Re-Use. Niskayuna, NY: Department of Energy, 2011.
44. ALTELA. *Oil and Gas Industry, Produced Water.* 2014. Available at <http://www.altelainc.com/applications/detail/oil-and-gas-industry-produced-water/>. Accessed on August, 2014.
45. US Environmental Protection Agency. *The Process of Hydraulic Fracturing.* 2014. Available at <http://www2.epa.gov/hydraulicfracturing/process-hydraulic-fracturing>. Accessed on August, 2014.
46. Zhong ZX, You FQ. Globally convergent exact and inexact parametric algorithms for solving large-scale mixed-integer fractional programs and applications in process systems engineering. *Comput Chem Eng.* 2014;61:90–101.
47. You F, Castro PM, Grossmann IE. Dinkelbach's algorithm as an efficient method to solve a class of MINLP models for large-scale cyclic scheduling problems. *Comput Chem Eng.* 2009;33:1879–1889.
48. You FQ, Wang B. Life Cycle Optimization of Biomass-to-Liquid Supply Chains with Distributed-Centralized Processing Networks. *Ind Eng Chem Res.* 2011;50:10102–10127.
49. You FQ, Tao L, Graziano DJ, Snyder SW. Optimal design of sustainable cellulosic biofuel supply chains: Multiobjective optimization coupled with life cycle assessment and input-output analysis. *AIChE J.* 2012;58:1157–1180.
50. Yue DJ, Guillen-Gosalbez G, You FQ. Global optimization of large-scale mixed-integer linear fractional programming problems: a reformulation-linearization method and process scheduling applications. *AIChE J.* 2013;59:4255–4272.
51. Charnes A, Cooper WW. Programming with linear fractional functionals. *Naval Res Logist Q.* 1962;9:181–186.
52. Glover F. Improved linear integer programming formulations of non-linear integer problems. *Manag Sci.* 1975;22:455–460.
53. Gupta OK, Ravindran A. Branch and bound experiments in convex nonlinear integer programming. *Manag Sci.* 1985;31:1533–1546.
54. Benichou M, Gauthier JM, Girodet P, Hentges G, Ribiere G, Vincent O. Experiments in mixed-integer linear programming. *Math Program.* 1971;1:76–94.
55. Mitra G. Investigation of some Branch And Bound strategies for the solution of mixed integer linear programs. *Math Program.* 1973;4: 155–170.
56. Lawler EL, Wood DE. Branch-And-Bound methods: a survey. *Oper Res.* 1966;14:699–719.
57. Ibaraki T. Theoretical comparisons of search strategies in branch-and-bound algorithms. *Int J Comput Inf Sci.* 1976;5:315–344.
58. Gong J, You F. Global optimization for sustainable design and synthesis of algae processing network for CO₂ mitigation and biofuel production using life cycle optimization. *AIChE J.* 2014;60:3195–3210.
59. Chu Y, You F. Integration of scheduling and control with online closed-loop implementation: fast computational strategy and large-scale global optimization algorithm. *Comput Chem Eng.* 2012;47: 248–268.
60. Chu Y, You F. Integration of production scheduling and dynamic optimization for multi-product CSTRs: generalized Benders decomposition coupled with global mixed-integer fractional programming. *Comput Chem Eng.* 2013;58:315–333.
61. Gong J, You F. Value-added chemicals from microalgae: greener, more economical, or both? *ACS Sustain Chem Eng.* In press. DOI: 10.1021/sc500683w.
62. Yue D, You F. Sustainable scheduling of batch processes under economic and environmental criteria with MINLP models and algorithms. *Comput Chem Eng.* 2013;54:44–59.
63. Yue D, Kim MA, You F. Design of sustainable product systems and supply chains with life cycle optimization based on functional unit: general modeling framework, mixed-integer nonlinear programming algorithms and case study on hydrocarbon biofuels. *ACS Sustain Chem Eng.* 2013;1:1003–1014.
64. Yue DJ, Slivinsky M, Sumpter J, You FQ. Sustainable design and operation of cellulosic bioelectricity supply chain networks with life cycle economic, environmental, and social optimization. *Ind Eng Chem Res.* 2014;53:4008–4029.
65. Tong KL, You FQ, Rong G. Robust design and operations of hydrocarbon biofuel supply chain integrating with existing petroleum refineries considering unit cost objective. *Comput Chem Eng.* 2014; 68:128–139.
66. Brooke A, Kendrick DA, Meeraus A, Rosenthal RE. *GAMS: A user's guide.* Course Technology, 1988.
67. Achterberg T. SCIP: solving constraint integer programs. *Math Program Comput.* 2009;1:1–41.
68. Tawarmalani M, Sahinidis NV. A polyhedral branch-and-cut approach to global optimization. *Math Program.* 2005;103:225–249.
69. USGS. *National Water Information System.* 2014. Available at <http://waterdata.usgs.gov/pa/nwis/current/?type=flow>. Accessed on September, 2014.
70. Arthur JD, Arthur R, Bohm B, Layne M, Shaieby T. Mixing and scale affinity model for hydraulic fracturing fluids. In: *International Petroleum and Bio-fuels Environmental Conference.* San Antonio, TX, 2010.
71. Jiang M, Hendrickson CT, VanBriesen JM. Life cycle water consumption and wastewater generation impacts of a marcellus shale gas well. *Environ Sci Technol.* 2014;48:1911–1920.
72. Clark C, Han J, Burnham A, Dunn J, Wang M. Life-cycle analysis of shale gas and natural gas. Argonne National Laboratory (ANL), 2012.
73. Maenza T, Posti J. Pennsylvania american water announces \$16.5 million investment to construct and rehab water storage tanks. Pennsylvania American Water, 2013.
74. Al-Nory MT, Brodsky A, Bozkaya B, Graves SC. Desalination supply chain decision analysis and optimization. *Desalination.* 2014; 347:144–157.
75. Utilities DW. *Average Costs Manual For Pipeline Construction Cost Estimation.* 2012.
76. Doran G, Leong LYC. Developing a cost effective environmental solution for produced water and creating a “new” water resource. Bakersfield, CA: U.S. Department of Energy, 2000.

Appendix A

In this section, we provide the input data of the Case Studies Section.

Parameter	Indices	Value	Unit
$CC_{i,j,t}$	—	100–200 ¹⁷	Mcf/bbl
CS_i	—	0.20–0.50 ¹⁴	\$/bbl
CI_i	—	100–140 ⁷³	\$/bbl
DR	—	0.10 ²⁸	annual
$FC_{i,c,m1,r}$	$r1$	15,800 ^{40,43}	\$
	$r2$	20,000 ^{40,43}	\$
	$r3$	23,800 ^{40,43}	\$
$FD_{i,d,m1,r}$	$r1$	238,000 ^{40,43}	\$
	$r2$	300,000 ^{40,43}	\$
	$r3$	357,000 ^{40,43}	\$
$FO_{i,o,q}$	$q1$	15,800 ^{27,74}	\$
	$q2$	20,000 ^{27,74}	\$
	$q3$	23,800 ^{27,74}	\$
$FR_{s,t}$	—	10,000–400,000 ^{14,69}	bbl/week
$FS_{s,i,m,r}$	$m1,r1$	158,000 ^{40,43}	\$
	$m1,r2$	200,000 ^{40,43}	\$
	$m1,r3$	238,000 ^{40,43}	\$
	$m2,r1$	986,000 ^{25,75}	\$
	$m2,r2$	1,500,000 ^{25,75}	\$
	$m2,r3$	1,910,000 ^{25,75}	\$
LC_i	$l1$	0.70 ^{27,43}	—
	$l2$	0.65 ^{27,43}	—
	$l3$	0.60 ^{27,43}	—
$LO_{l,o}$	$o1$	1.00 ^{27,43}	—
	$o2$	0.98 ^{27,43}	—
	$o3$	0.70 ^{27,43}	—
$MC_{i,c,m1,r}$	$r1$	30,000 ^{14,43}	bbl
	$r2$	45,000 ^{14,43}	bbl
	$r3$	60,000 ^{14,43}	bbl
$MD_{i,d,m1,r}$	$r1$	30,000 ^{14,43}	bbl
	$r2$	45,000 ^{14,43}	bbl
	$r3$	60,000 ^{14,43}	bbl
$MS_{s,i,m,r}$	$m1,r1$	30,000 ^{14,43}	bbl
	$m1,r2$	45,000 ^{14,43}	bbl
	$m1,r3$	60,000 ^{14,43}	bbl
	$m2,r1$	200,000 ⁷⁵	bbl
	$m2,r2$	400,000 ⁷⁵	bbl
	$m2,r3$	600,000 ⁷⁵	bbl
RF_o	$o1$	5.67 ^{27,76}	—
	$o2$	1.86 ^{27,76}	—
	$o3$	0.25 ^{27,76}	—
$RW_{i,j,t}$	—	300–500 ¹⁷	bbl/week
SC_i	—	15,000–25,000 ⁷³	bbl
SM_i	—	50,000–80,000 ⁷³	bbl
$SP_{i,t}$	—	0.10–1.00 ⁴⁰	\$/Mcf
$TC_{i,c,m1}$	—	0.60–3.00 ^{25,40}	\$/bbl
$TD_{i,d,m1}$	—	9–18 ^{25,40}	\$/bbl
$TS_{s,i,m}$	$m1$	0.2–1.0 ^{25,40}	\$/bbl
	$m2$	0.01–0.03 ^{25,40}	\$/bbl
$VC_{i,l,c,t}$	$l1$	1.00–2.20 ^{25,27}	\$/bbl
	$l2$	2.50–2.95 ^{25,27}	\$/bbl
	$l3$	2.75–5.00 ^{25,27}	\$/bbl
$VD_{i,l,d,t}$	—	0.80–1.20 ^{25,39}	\$/bbl
$VO_{i,l,o,t}$	$l1,o1$	1.60 ^{27,43}	\$/bbl
	$l1,o2$	2.00 ^{27,43}	\$/bbl
	$l1,o3$	4.50 ^{27,43}	\$/bbl
	$l2,o1$	1.80 ^{27,43}	\$/bbl
	$l2,o2$	3.00 ^{27,43}	\$/bbl
	$l2,o3$	5.00 ^{27,43}	\$/bbl
	$l3,o1$	2.00 ^{27,43}	\$/bbl
	$l3,o2$	3.50 ^{27,43}	\$/bbl
	$l3,o3$	6.50 ^{27,43}	\$/bbl
WA_s	—	0.04–0.06 ²⁵	\$/bbl
$WC_{c,t}$	—	6,000–20,000 ²⁷	bbl/week
$WD_{d,t}$	—	1,000–5,000 ²⁷	bbl/week
$WO_{i,o,q}$	$o1,q1$	5,000 ^{27,43}	bbl/week
	$o1,q2$	10,000 ^{27,43}	bbl/week
	$o1,q3$	15,000 ^{27,43}	bbl/week

(Continued)

Table (Continued)

	$o2,q1$	1,000 ^{27,43}	bbl/week
	$o2,q2$	2,000 ^{27,43}	bbl/week
	$o2,q3$	4,000 ^{27,43}	bbl/week
	$o3,q1$	5,000 ^{27,43}	bbl/week
	$o3,q2$	10,000 ^{27,43}	bbl/week
	$o3,q3$	20,000 ^{27,43}	bbl/week
$WP_{i,j,l,t}$	$l1$	5–9 ^{26,43}	bbl/week
	$l2$	10–20 ^{26,43}	bbl/week
	$l3$	45–105 ^{26,43}	bbl/week

Appendix B

In this section, we present the supplemental computational studies to demonstrate the efficiency of proposed solution methods, details of which are given as the following.

The general form of MILFP problem is given as the following problem (TP),

$$\begin{aligned}
 (TP) \quad & \max \frac{A_0 + \sum_{i \in I} A_{1,i}x_i + \sum_{j \in J} A_{2,j}y_j}{B_0 + \sum_{i \in I} B_{1,i}x_i + \sum_{j \in J} B_{2,j}y_j} \\
 \text{s.t.} \quad & \sum_{i \in I} C_{1,i,k}x_i + \sum_{j \in J} C_{2,j,k}y_j \leq D_k, \quad \forall k \in K \\
 & B_0 + \sum_{i \in I} B_{1,i}x_i + \sum_{j \in J} B_{2,j}y_j > 0 \\
 & x^L \leq x_i \leq x^U, \quad \forall i \in I \text{ and } y_j \in \{0, 1\}, \quad \forall j \in J
 \end{aligned}$$

We note that all constraints are linear and the objective function is formulated as a ratio of two linear functions. Such a problem consists of $|I|$ continuous variables, $|J|$ binary variables, and $|K|+1$ constraints. This additional constraint is the second constraint, which is used to guarantee that the denominator of the original objective function is positive. The value of $|I|$, $|J|$ and $|K|$ ranges from 15 to 3,000. we solve 50 randomly generated instances to illustrate the computational efficiency of the aforementioned algorithms, including the proposed Branch-and-Bound algorithm, the parametric algorithm, and the reformulation-linearization algorithm, as well as general MINLP solution methods, that is, DICOPT (outer-approximation), SBB (simple Branch-and-Bound algorithm), and global optimizers BARON 12 and SCIP 3.

The performance profiles of solving the MILFP test problem (TP) are given in Figure B1, based on the performance analysis and benchmarking methods of optimization algorithms. In this figure, the x -axis is the maximum computational time needed for solving a problem, and the y -axis is the number of instances that can be solved within that time. Therefore, if one solution method has a performance profile approaching the upper left corner, it means this method can solve more problems within a shorter time. In other words, it has high computational efficiency.

From this figure, we can see that the computational performances of the parametric algorithm and reformulation-linearization algorithm obviously surpass those of the tested general-purpose MINLP solvers in solving the MILFP problems. The reformulation-linearization algorithm performs slightly better than the parametric algorithm. The proposed Branch-and-Bound and Charnes–Cooper algorithm shows a relatively stable performance. Although in the beginning, it falls behind the DICOPT and SBB solvers, which means that it does not solve

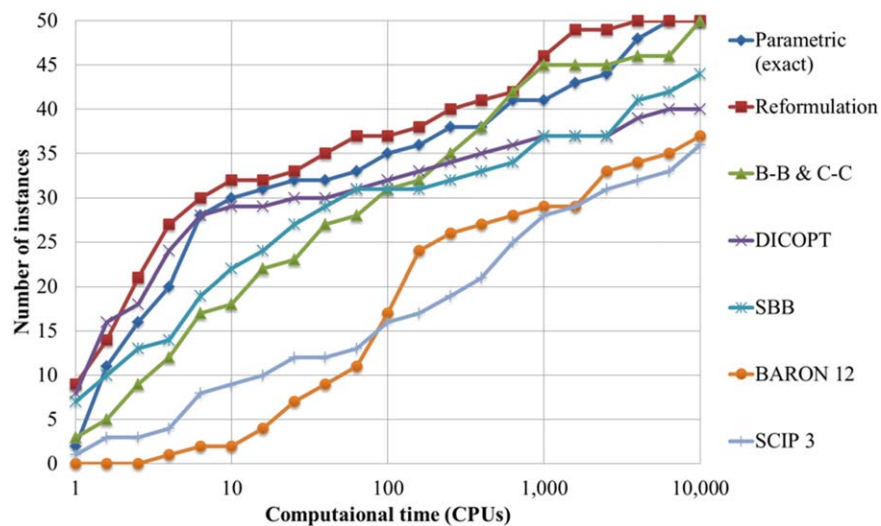


Figure B1. Performance profile for the solution of the 50 instances of MILFP testing problem.

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

some small instances efficiently enough due to the branching process. When given a longer computational time, that is, solving large-scale problems, it solves more instances than general-purpose MINLP solvers and is close or even outperforms the parametric algorithm and reformulation-linearization algorithm. We also note that DICOPT, SBB, BARON 12, and SCIP 3 fail to solve certain instances due to either solver errors or low computational efficiency. Meanwhile, due to the Branch-and-Bound scheme applied in the Branch-and-Bound and Charnes–Cooper

algorithm, it returns feasible solution to all the 50 instances within the given time limits. The parametric algorithm and reformulation-linearization algorithm are both efficient approaches, and the newly proposed Branch-and-Bound and Charnes–Cooper algorithm emerges as a promising solution option for solving large-scale MILFP problems with global optimality.

Manuscript received Sep. 8, 2014, and revision received Nov. 13, 2014.