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Evaluating the spatiotemporal variability of water recovery ratios of shale gas wells and their effects on shale gas development

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ABSTRACT

Unconventional shale gas production in the United States has been largely improved due to the development of hydraulic fracturing technology and is projected to rapidly grow in the coming years. However, the acquisition of freshwater and management of flowback and produced (FP) water associated with hydraulic fracturing operation are two of the greatest challenges in shale gas development, especially in arid regions. For efficient and sustainable water management, a better understanding of freshwater consumption and FP water production for shale gas wells is necessary to appropriately expand and upgrade the existing water network and shale gas network. To achieve this, we first collected water-use volume and monthly FP water production volume data for shale gas wells drilled in the Eagle Ford and Marcellus shale regions. Next, after integrating the data from multiple database sources, the water recovery ratio was calculated as the ratio of cumulative FP water volume to water-use volume and used as a metric to characterize the wells in these two shale regions. Then, we analyzed the obtained water recovery ratio data according to the location and production history to study the spatiotemporal variations across multiple counties and time periods. It shows that around 30% of the collected wells drilled in the Eagle Ford region have the water recovery ratio greater than 1; however, only 1% of the collected wells drilled in the Marcellus region have the water recovery ratio greater than 1. Besides, the water recovery ratios vary significantly across the counties in each shale region. To demonstrate how different water recovery ratio may affect shale gas development, a shale gas supply chain network (SGSCN) optimization model from the literature was utilized to perform two case studies in the Marcellus region. The optimal results suggest that different configurations of SGSCN are required for economically desirable and practically feasible management of shale gas wells with different water recovery ratios.

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1. Introduction

Natural gas is one of the most important energy sources used to meet the global energy demand. In recent years, with constantly developing horizontal drilling and hydraulic fracturing technologies, shale gas production has been significantly improved by extracting shale gas trapped in tight formation and has become the main contributor to the total natural gas supply in the United States (EIA, 2018). This “shale revolution” has created tremendous opportunities for monetization into value-added fuels and chemicals (Al-Douri et al., 2017) and has also triggered rapid rise of drilling of unconventional shale gas wells all over the world (Freyman, 2014; Vengosh et al., 2014; Yu et al., 2016). Such enhanced levels of production have generated great concerns and intense debates on the accompanying environmental implications, especially regarding the amount of freshwater required for hydraulic fracturing operation, and management of wastewater generated along with shale gas production (Akob et al., 2016; Freyman, 2014; Scanlon et al., 2014; Veil, 2015).

Hydraulic fracturing operation requires large amounts of

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freshwater for its successful implementation. For a typical shale gas well, around 3–7 million gallons of freshwater are injected with proppant (mostly sand) and chemical additives under high pressure to break rock formation and form high-permeability pathways for gas extraction (Lira-Barragán et al., 2016). Hydraulic fracturing process is generally completed within 2–3 days, and the amount of water to be injected must be supplied within such a short period of time (Dunn, 2016). Even though previous studies have presented that the water supply for hydraulic fracturing process accounts for only a small fraction of the overall industrial water use in the United States (Ikonnikova et al., 2017; Kondash and Vengosh, 2015; Kondash et al., 2018), it still can lead to a gap between local water demand and supply, particularly in water-scarce regions (Kondash et al., 2017; Scanlon et al., 2014, 2017; Vengosh et al., 2014). Thus, understanding the required water-use volume and the water availability on a local scale is important to planning hydraulic fracturing practices and designing water supply network.

During and after the completion of hydraulic fracturing operation, some of the injected fracturing fluid returns to the surface due to the decreasing wellbore pressure and high natural stress in rock formations. Meanwhile, some formation water (i.e., naturally occurring water entrapped in pore spaces in shale formation) with high salinity also flows from the matrix into the fractures and then returns to the surface along with shale gas production. Thus, the generated wastewater consists of a combination of the injected fracturing fluid and formation brine, where the proportion of the formation brine increases drastically over time (Kondash and Vengosh, 2015). This increasing contribution of the formation brine results in an increase in the overall salinity of the wastewater and concentration of various contaminants (e.g., total dissolved solids (TDS), total suspended solids (TSS), metals, naturally occurring radioactive material (NORM), organics and hydrocarbons), which may lead to major environmental issues (Warner et al., 2013; Yang et al., 2014). Generally, the wastewater is called flowback and produced (FP) water. The difference between flowback and produced water is time spent in the well; specifically, most flowback water is generated within the first few weeks (i.e., up to about 2 months), while produced water refers to the wastewater that returns thereafter, throughout the entire lifespan of the shale well. However, even though a detailed chemical analysis may help distinguish between flowback and produced water, the time point of transition from flowback water to produced water is usually hard to discern. Thus, in many database sources, the combined FP water production volume data are usually reported without a specific distinction between flowback and produced water. Regarding the FP water production associated with shale gas development, previous studies have suggested that with more water being used for hydraulic fracturing operations, more FP water is being generated, and thus expanded and upgraded wastewater management system is required (Ikonnikova et al., 2017). Conventional disposal option to inject FP water into deep wells has become less applicable since it may cause seismicity, contamination of surface water, and high transportation cost if disposal wells are not available near drilling sites (Yang et al., 2015). However, applying advanced treatment technology to handle the large amount of FP water for safe release is generally energy-intensive and expensive (Elsayed et al., 2014; Ikonnikova et al., 2017). Furthermore, in different shale regions, the amount of FP water production, and the type and concentration of contained contaminants can be largely different, which makes the design work even more complicated. Thus, it is necessary to develop an economically viable and environmentally sustainable wastewater management strategy directly based on the quantity and quality of produced FP water on a local scale.

Many research activities have incorporated process systems engineering (PSE) approaches to address the challenges associated with strategic planning, scheduling, and process control of shale gas development. A complete review on design and optimization of shale gas energy systems can be found in the work of Gao and You (2017). Cafaro and Grossmann (2014) first presented a large-scale mixed-integer nonlinear programming (MINLP) model for the long-term planning of shale gas supply chain, to maximize the overall economic performance. This work was extended by Drouven and Grossmann (2016) to explicitly consider the spatial variation in shale gas composition. Since design and operational decisions associated with the hydraulic fracturing water cycle are increasingly important, Yang et al. (2014) developed a modeling framework to optimize water-use life cycle for shale gas water management, which was further extended to capture the investment decisions associated with water management (Yang et al., 2015). Gao and You (2015a) proposed a mixed-integer linear fraction programming (MILFP) model to specifically address the optimal design and operations of water supply chain networks for shale gas development, where various water management options were considered. To integrate the design of shale gas supply chain and water management, Guerra et al. (2016) proposed an optimization framework for the techno-economic evaluation of the integrated network. Oke et al. (2019) developed a mathematical framework to optimize water-energy nexus, where a detailed design model of membrane distillation (MD) was implemented to capture the energy-related decisions. Taking the greenhouse gas (GHG) emissions into account, Gao and You (2015b) performed a comprehensive framework to address the life cycle economic and environmental optimization of shale gas supply chain network. Chen et al. (2017) also proposed an LCA-based multi-level decision-making programming approach to consider conflicting goals from different decision makers. Furthermore, the uncertainty in freshwater availability (Guerra et al., 2019; Yang et al., 2014), estimated ultimate recovery (EUR) (Gao and You, 2015c), hydraulic fracturing water usage and flowback water generation (Guerra et al., 2019; Lira-Barragán et al., 2016), wastewater quality (Guerra et al., 2019), shale gas production (Drouven et al., 2017; Guerra et al., 2019), prices of natural gas and natural gas liquids (LNGs) products (Chebeir et al., 2017; Drouven et al., 2017; Li et al., 2020), and solar energy availability and fossil fuels price (Al-Aboosi and El-Halwagi, 2019) were considered and discussed in the shale gas supply chain design. In recent years, several studies have developed dynamic model identification frameworks for hydraulic fracturing process (Narasingam et al., 2017; Narasingam and Kwon, 2017, 2018) and optimal pumping schedules to achieve desired fracture geometry and uniform proppant distribution for enhanced shale gas recovery (Siddhamshetty et al., 2018, 2019; Siddhamshetty and Kwon, 2019). Based on these, the pumping schedule design for hydraulic fracturing operation was successfully integrated with shale gas water management (Cao et al., 2019; Etoughe et al., 2018) and shale gas supply chain network (Ahn et al., 2019, Ahn et al., 2020). In addition, Asala et al. (2019) and Chebeir et al. (2019) proposed a data-driven techno-economic framework for shale gas supply chain design, where reservoir simulation was integrated to determine the gas and water production profiles, and machine learning techniques were integrated to predict water availability, products prices, and market demands. To accomplish these studies, the volumes of injected water and generated FP water are required as necessary input data to their optimization models. However, most of the used data were either collected from a few specific wells drilled in a relatively narrow region or generated using simple empirical models developed based on limited data. Since the design decisions can be significantly affected by the water-use and FP water volumes, appropriate modification of the optimal design of shale gas supply chain and water management becomes essential to deal with spatiotemporal variability in water-use and FP water volumes

(Mauter et al., 2014). In this regard, some attempts have been made recently to evaluate the water injected for hydraulic fracturing operation and the associated FP water production in major unconventional shale gas and oil regions (Ikonnikova et al., 2017; Kondash and Vengosh, 2015; Kondash et al., 2018; Scanlon et al., 2014). In these studies, wide ranges of water-use and FP water volumes were provided for specific shale formations. For the purpose of presenting the water footprint of hydraulic fracturing process, a metric called water intensity (i.e., the amount of water required to produce a unit volume of gas or energy) was generally used to normalize the water data and compare it with other energy-producing materials. However, only few studies had a thorough discussion on the significance of water recovery ratio, which is defined as the ratio of the FP water volume to the corresponding water-use volume, to efficient and sustainable water management. Specifically, a greater water recovery ratio implies that more FP water will be produced for a given amount of injected water, which indicates that more treated water can be reused for future hydraulic fracturing operations in the same shale site and even the other shale sites with high water demand, or recycled for agricultural purposes and industrial uses; as a result, there will be much less stress on the freshwater supply. As the wells with different water recovery ratios may require different water management strategies, obtaining preliminary knowledge about the water recovery ratio is critical for evaluation of FP water production and thus for greener shale gas production.

Motivated by these considerations, the objective of this study is to evaluate the water recovery ratio in different shale formations. Water-use volume and FP water production volume data for the wells drilled in the Eagle Ford and Marcellus regions were collected from multiple database sources, including the FracFocus Chemical Disclosure Registry 2.0, the DrillingInfo Desktop application, and the gas and oil reporting website of the Pennsylvania Department of Environmental Protection. Then, utilizing the collected water-use and FP water production data, we calculated the corresponding water recovery ratio for each specific well drilled in both the target shale regions, which were then analyzed spatiotemporally to present the underlying variations across multiple regions and time periods. Finally, a shale gas supply chain network (SGSCN) optimization model was applied to demonstrate that different optimal network designs and configurations are required for the regions with different water recovery ratios. The spatiotemporal analysis of the water recovery ratio data will help provide a foundation for researchers and industry professionals to access, design and implement better water management practices for shale gas development.

2. Material and methodology

The goal of this study is to evaluate the water recovery ratios of shale gas wells drilled in different shale regions. We first collected the water-use and FP water production data for each of the available shale gas wells in the Eagle Ford and Marcellus shale regions using multiple database sources, and then performed data processing to calculate the corresponding water recovery ratio. The flow diagram is shown in Fig. 1. Once the water recovery ratio data were obtained, their spatiotemporal characteristics were analyzed, and used for SGSCN design.

2.1. Data sources

The FracFocus Chemical Disclosure Registry 2.0 (FracFocus, 2019) was used to collect water-use data for hydraulic fractured wells in the United States. The reported “total base water volume”, which was taken as the water-use volume in this study, refers to the volume of water used as a carrier fluid (i.e., water and sand make up 98−99.5% of hydraulic fracturing fluid). Note that in this database, well orientation of each reporting well as well as shale formation where the well was drilled is not reported. On the other hand, the DrillingInfo Desktop application (DrillingInfo, 2019) provides cumulative production volumes of gas, oil and FP water for wells in the major unconventional gas and oil formation in the United States. In the case of some shale formations (e.g., the Fayetteville, Marcellus and Woodford formation), FP water production volumes are not available from the DrillingInfo, and thus, these data should be collected from other sources. For example, the FP water production volumes in the Marcellus region can be collected from the gas and oil reporting website of the Pennsylvania Department of Environmental Protection (PA DEP, 2019). Note that in this database, the cumulative FP water production volumes are not directly posted but can be calculated by integrating the provided monthly production data.

2.2. Data processing

To calculate the water recovery ratios of shale gas wells, it requires integration of multiple database sources to obtain the water used for hydraulic fracturing operation and FP water produced along with shale gas production for individual wells. In this study, since we mainly focused on the shale gas wells drilled in the Eagle Ford region in Texas and the Marcellus region in Pennsylvania since 2009, the water-use data were collected from the FracFocus database, while the cumulative FP water production data were downloaded from the DrillingInfo and PA DEP databases. Since most of the available wells in the Marcellus region are horizontally drilled unconventional gas wells, the collected water data from the Eagle Ford region were further filtered by primary production type (i.e., gas) and drilling type (i.e., horizontal drilling). Unlike the PA DEP database, the DillingInfo database does not provide any information that can be used to judge whether the horizontally drilled wells in the Eagle Ford region are unconventional. Note that the wells with null or zero value in either water-use volume or cumulative FP water production volume were removed manually before conducting the subsequent data matching process. Then, to match the water-use volume with the corresponding cumulative FP water production volume for each well, we used American Petroleum Institute (API) number to organize the collected data, which is available in all the databases and can be used for well identification. Finally, the matched water data were used to calculate the corresponding water recovery ratios, which is defined as follows:

$$R_{n,t} = V_{n,t}^{pro} \Big/ V_{n}^{inj} \quad (1)$$

where V_n^{inj} is the water-use volume injected for shale gas well n, $V_{n,t}^{pro}$ is the cumulative FP water production volume over t months since its first production date for shale gas well n, and $R_{n,t}$ is the corresponding water recovery ratio of shale gas well n over n months since its first production date. Thus, the water recovery ratio is specific to the considered production history and each specific well may have multiple water recovery ratios. In this study, we mainly considered the water recovery ratio calculated using the cumulative FP water production volume over the entire production history of each well.

Some additional information was also obtained from the databases. Specifically, geolocation information (i.e., latitude and longitude coordinate, county, and state) is available in all databases, and thus, the exact location for each well can be described in the shale regions. In this study, we used the coordinates collected from the DrillingInfo database and the PA DEP database to locate the

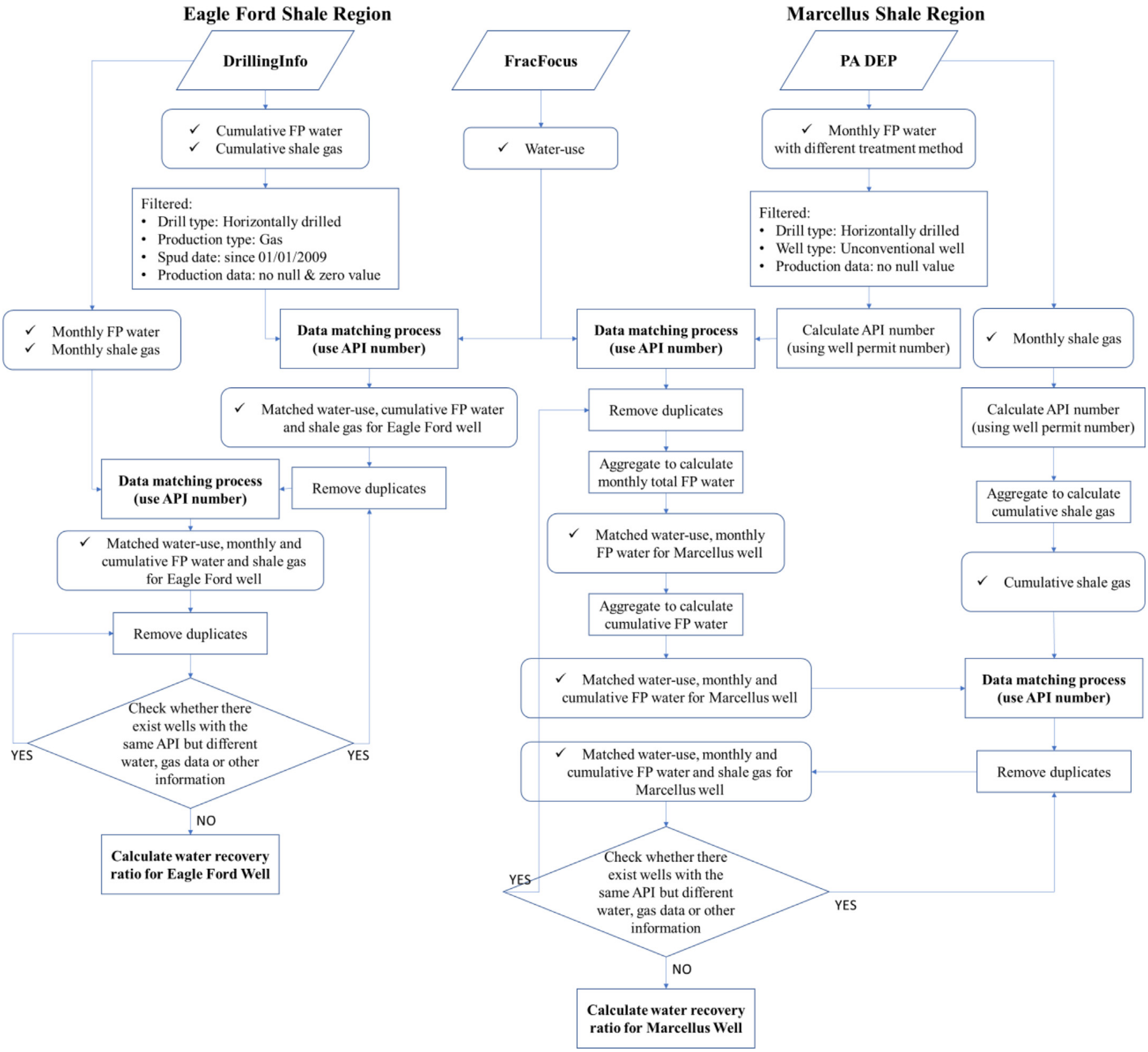


Fig. 1. Flow diagram of data collection and processing.

wells drilled in the Eagle Ford and Marcellus regions respectively, as presented in Fig. 2.

After the integration of databases, temporal information of each well was also recorded, including spud date (i.e., the date when drilling commenced), hydraulic fracturing job start/end data (i.e., the date when hydraulic fracturing operation started/ended), completion date (i.e., the date when the well was completed), and first/last production date (i.e., the first/last date when the production data were reported). For some of the collected wells, there exists a gap between the completion date and the first production date, which could be due to many reasons, such as no production during the period, reporting error, or missing data. In this study, the first production date ($t_n^{first\ prod}$) and last production date ($t_n^{last\ prod}$) were used to calculate the production period (T_n; i.e., the length of entire production history) for well n, which is defined in Equation (2).

$$T_n = t_n^{last\ prod} - t_n^{first\ prod} \tag{2}$$

Note that most of the wells considered for data collection are still active in FP water production, and thus, more precisely speaking, $t_n^{last\ prod}$ indicates the last date for which the FP production data is available for well n.

To apply shale gas supply chain optimization model, the corresponding gas and oil production data for each well were also collected from the DrillingInfo and the PA DEP databases. Since shale gas is the main products in the target wells, we only considered the gas production data for the subsequent analysis, even though they may also have other condensate or oil production reported. It should be noted that in the PA DEP database, the shale gas production data and FP water production data are provided in separated files, which also requires the data matching process

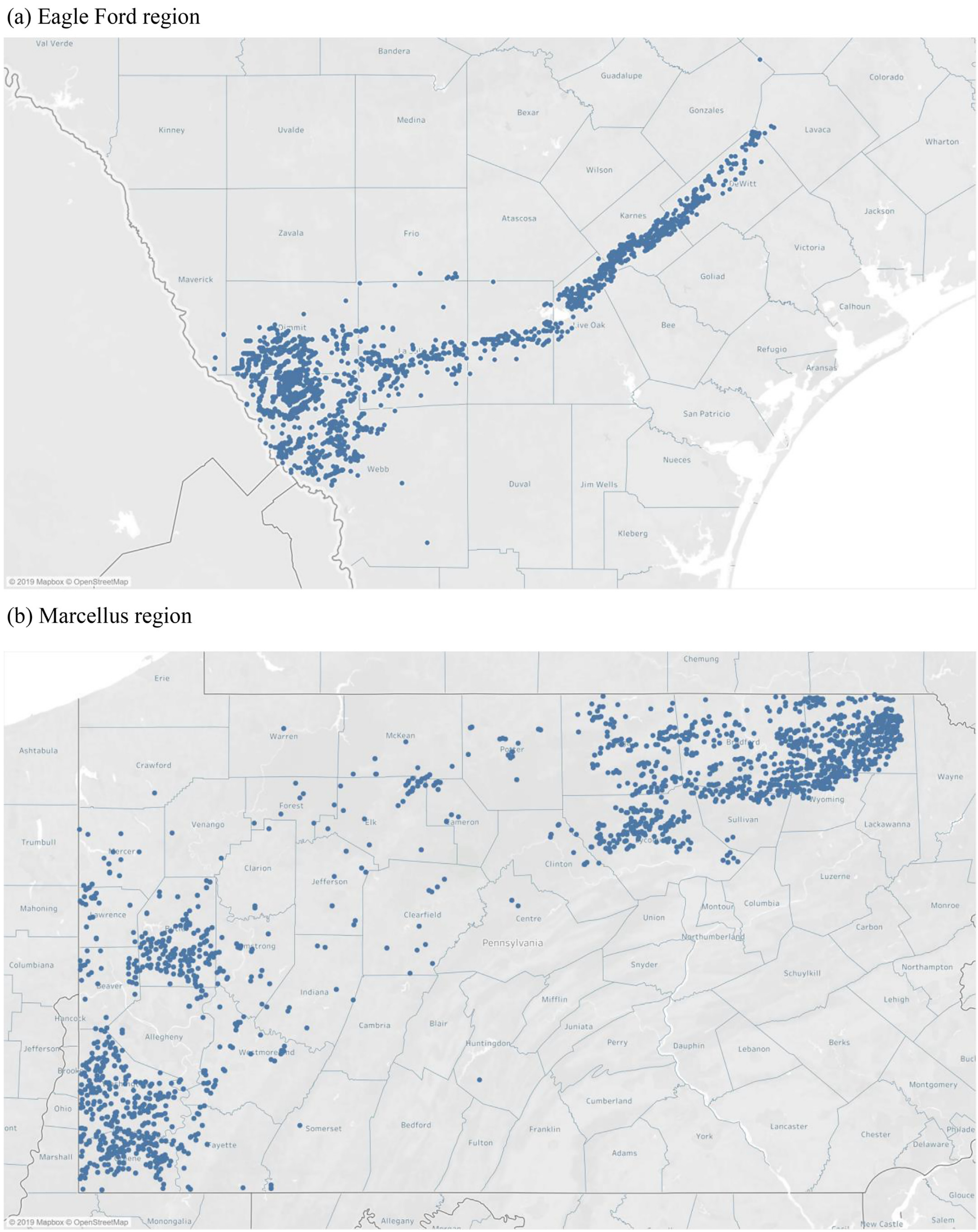


Fig. 2. Available shale gas wells in the (a) Eagle Ford region and (b) Marcellus region.

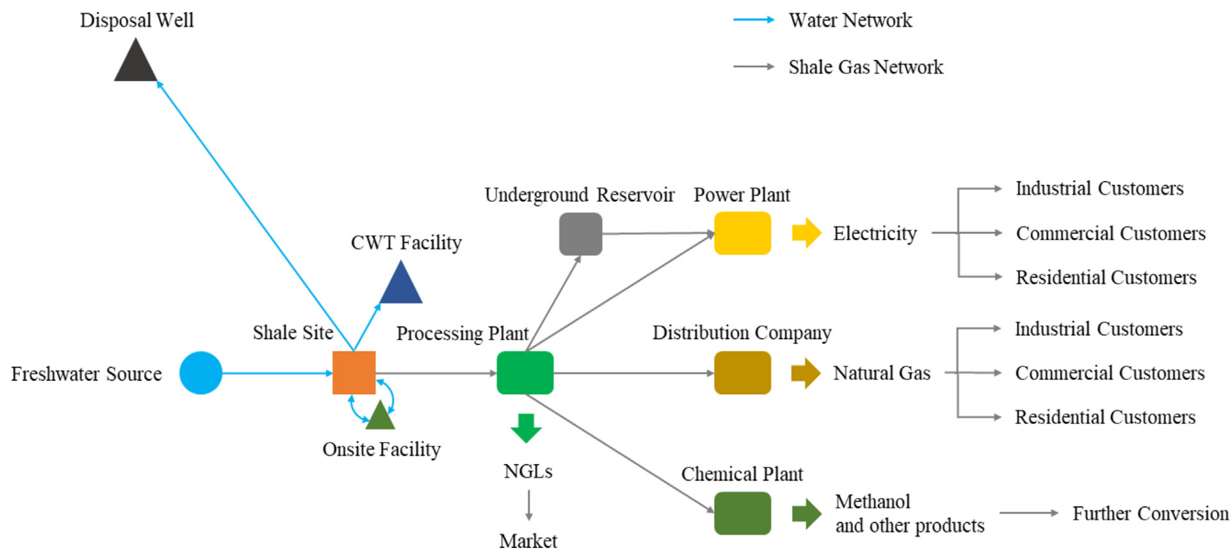


Fig. 3. Superstructure of shale gas supply chain network.

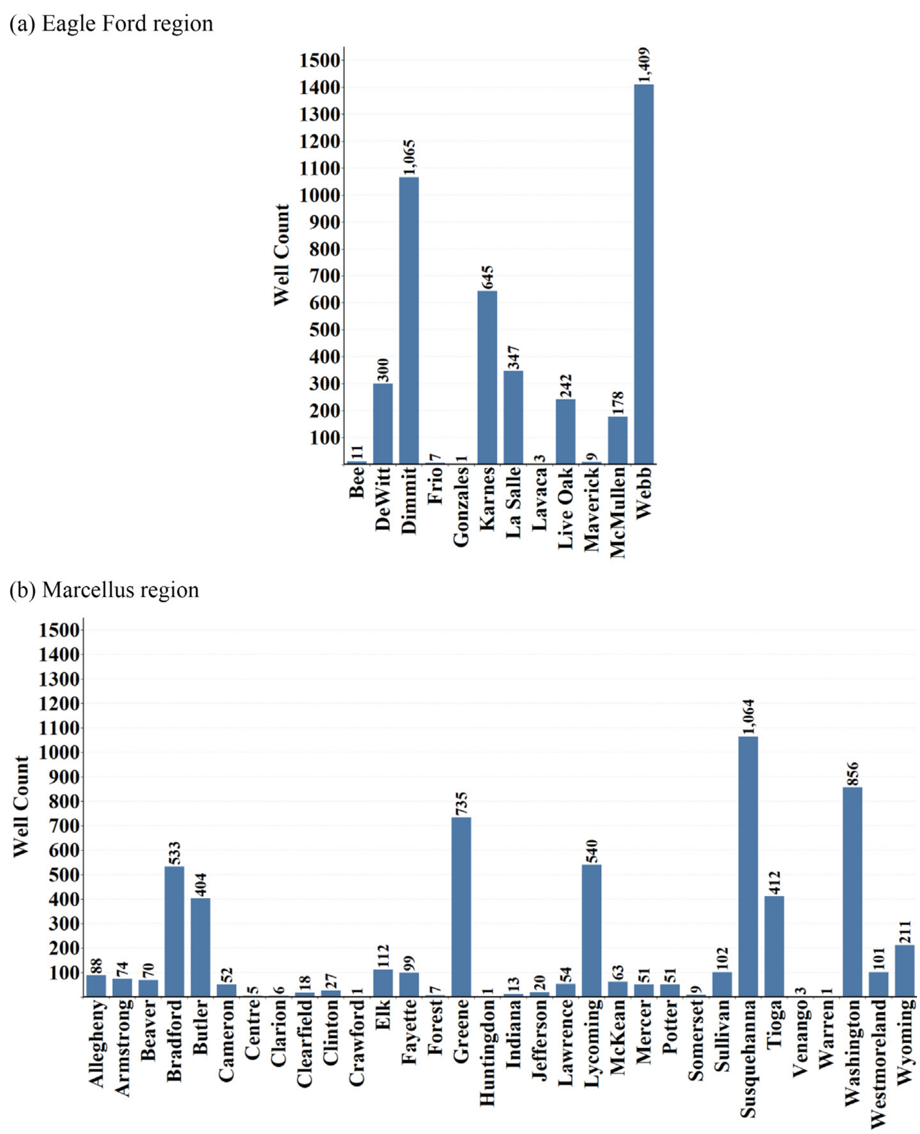


Fig. 4. Well count in each county in the (a) Eagle Ford region and (b) Marcellus region.

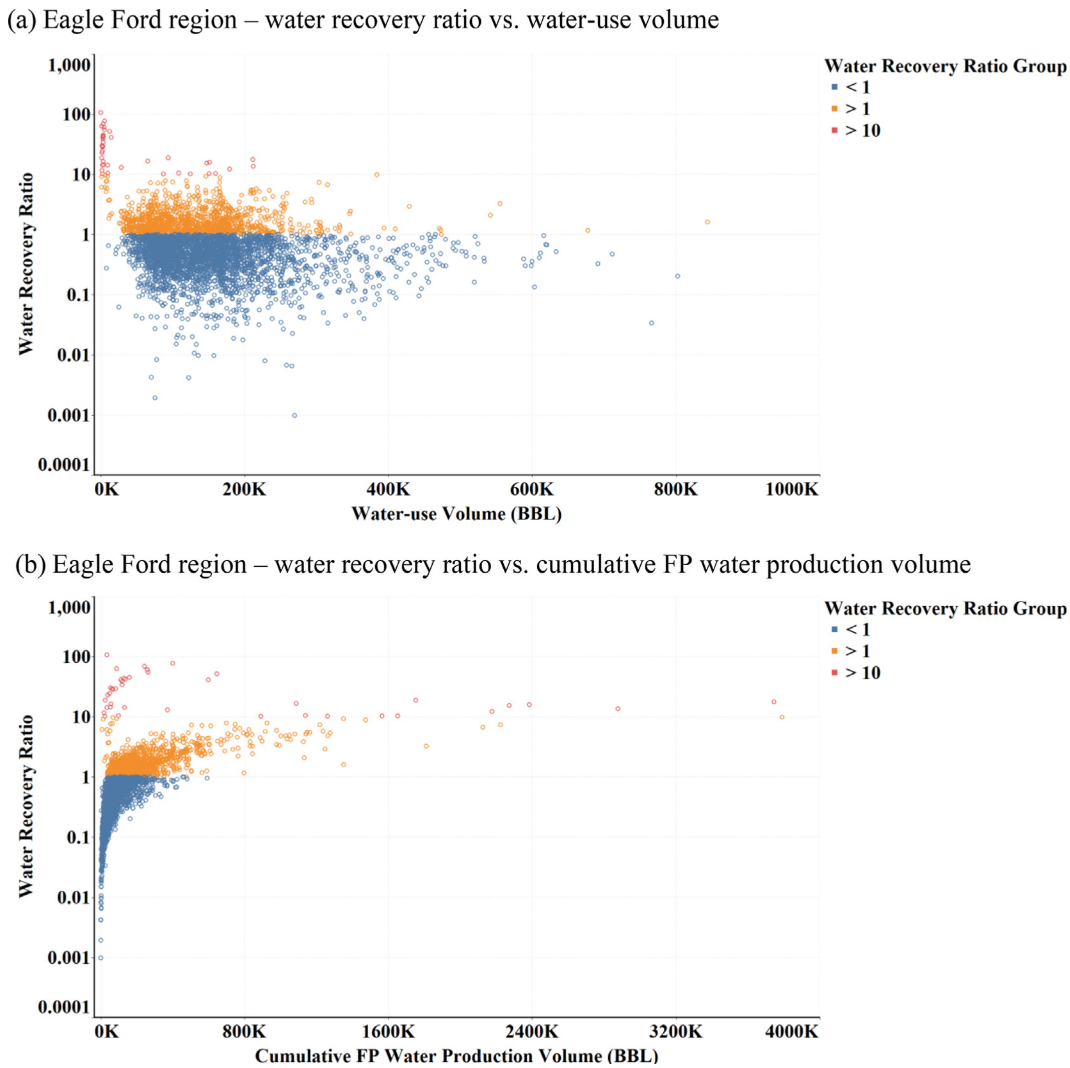


Fig. 5. Relations between the water recovery ratio and the corresponding (a) water-use volume and (b) cumulative FP water production volume in the Eagle Ford region; relations between the water recovery ratio and the corresponding (c) water-use volume and (d) cumulative FP water production volume in the Marcellus region.

using the API number. Besides, the first production dates of shale gas and FP water for individual wells can be different since some FP water may flow back to the surface prior to shale gas production (i.e., flowback water before well completion).

2.3. Shale gas supply chain network

To demonstrate how the water recovery ratio affects the design and configuration of shale gas supply chain network (SGSCN), the optimization model developed by Ahn et al. (2019) was applied. A general shale gas supply chain network is presented in Fig. 3, which can be roughly divided into the water network and shale gas network. Specifically, in the water network, the injected water required for drilling and hydraulic fracturing operation in shale sites can be obtained from freshwater sources (i.e., freshwater) and onsite treatment facilities (i.e., reused water). When hydraulic fracturing operation is completed, the generated FP water can be injected into disposal wells, treated by centralized wastewater treatment (CWT) facilities, or treated by onsite treatment facilities. Note that the treated water from the CWT facilities is directly discharged to surface water, while the one from the onsite treatment facilities is mixed with some freshwater and then reused for the other hydraulic fracturing operations in the same shale site. In the shale gas network, shale gas produced from shale sites is transported to processing plants for separation into natural gas (i.e., methane) and natural gas liquids (NGLs; i.e., ethane, propane, butane, etc.). Note that the separated NGLs are sold in the market as valuable by-products while the natural gas can be supplied to power plants for electricity generation, distribution companies for direct selling or export, and chemical plants for conversion and further processing to obtain various products (e.g., methanol, DME, olefins, and etc.) (Elbashir et al., 2019).

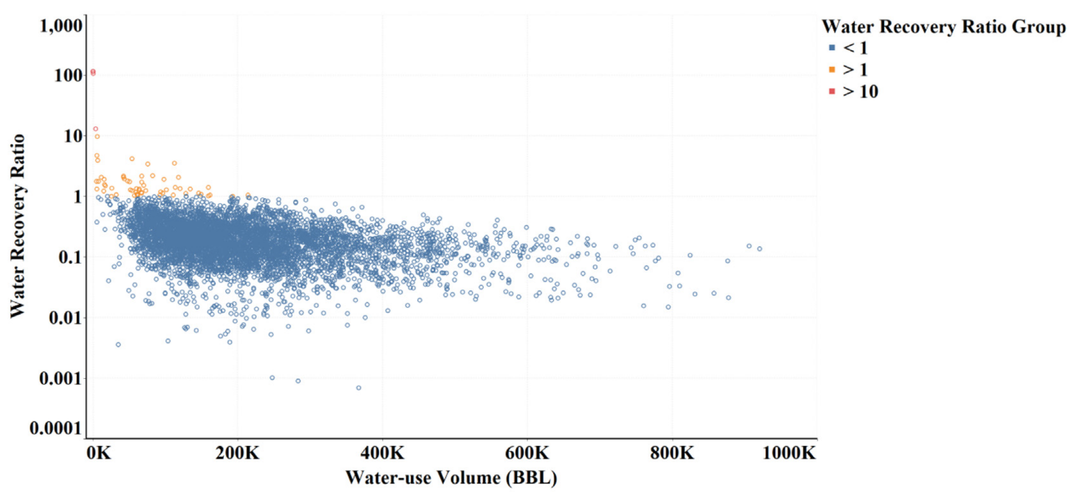
Since the power plant sector accounts for the highest monetization of natural gas compared to others, we assumed the power plant as the only monetization of the obtained natural gas in this study. Thus, the SGSCN considered includes freshwater acquisition, shale well drilling and hydraulic fracturing, wastewater management, shale gas processing, electricity generation, transportation system, and storage facility. Note that in the SGSCN optimization model, the change in TDS concentration of the FP water was not considered. Thus, the necessary inputs to this SGSCN model are water-use volume, FP water production and shale gas production profiles for each well in the shale sites. To demonstrate the significance of different water recovery ratios to the optimal design and configuration of SGSCN, we considered two groups of wells in the Marcellus region, whose water recovery ratios are largely different; the design parameters for facilities associated with the SGSCN were taken from the literature (Ahn et al., 2019; Gao and You, 2015b).

3. Results and discussion

The data of 4217 and 5783 wells in the Eagle Ford region and the Marcellus region were collected, respectively. The production period of these wells varies from less than one year to more than ten years, and most of the wells were still under production in 2018. As presented in Fig. 2, these wells are not evenly distributed in both shale regions; the number of collected wells in each county is presented in Fig. 4, which reiterates the distributed nature of the wells.

For these wells, we calculated the water recovery ratios using the water-use and cumulative FP water production volumes, which are presented in Fig. 5. We observed a huge difference in water recovery ratio between the Eagle Ford and Marcellus regions. Specifically, 70% of the collected wells drilled in the Eagle Ford region have the water recovery ratio less than 1; while, 99% of the collected wells drilled in the Marcellus region have the water recovery ratio less than 1, and 75% of them have the water recovery ratio less than 0.3. Since the produced water is mainly composed of formation brine trapped in underground formations, the volume of produced water that is allowed to flow back to the surface depends on the formation characteristics. Thus, there is possibility that the cumulative FP water production volume can be greater than the injected water volume, especially when the propagated fractures are in contact with nearby water-bearing formation. In this case, the resulting water recovery ratio is greater than 1. As reported, the Eagle Ford region is identified as the relatively desiccated formation while the Marcellus region is highly desiccated formations (Mantell, 2011); in other words, more formation brine can be generated along with oil and gas in the Eagle Ford region than the Marcellus region. Thus, it makes sense to observe that the water recovery ratios of the wells in the Eagle Ford region are typically greater than the ones in the Marcellus region. Besides, the red circles in Fig. 5 indicate that there are some outliers in both the shale regions whose water recovery ratios are even greater than 10. These outliers are attributed to either extremely small water-use volumes (Fig. 5(a) and (c)) or relatively large cumulative FP water production volumes (Fig. 5(b) and (d)). Similarly, it shows that there are also some wells with extremely low water recovery ratios

(c) Marcellus region – water recovery ratio vs. water-use volume



(d) Marcellus region – water recovery ratio vs. cumulative FP water production volume

Fig. 5. (*continued*).

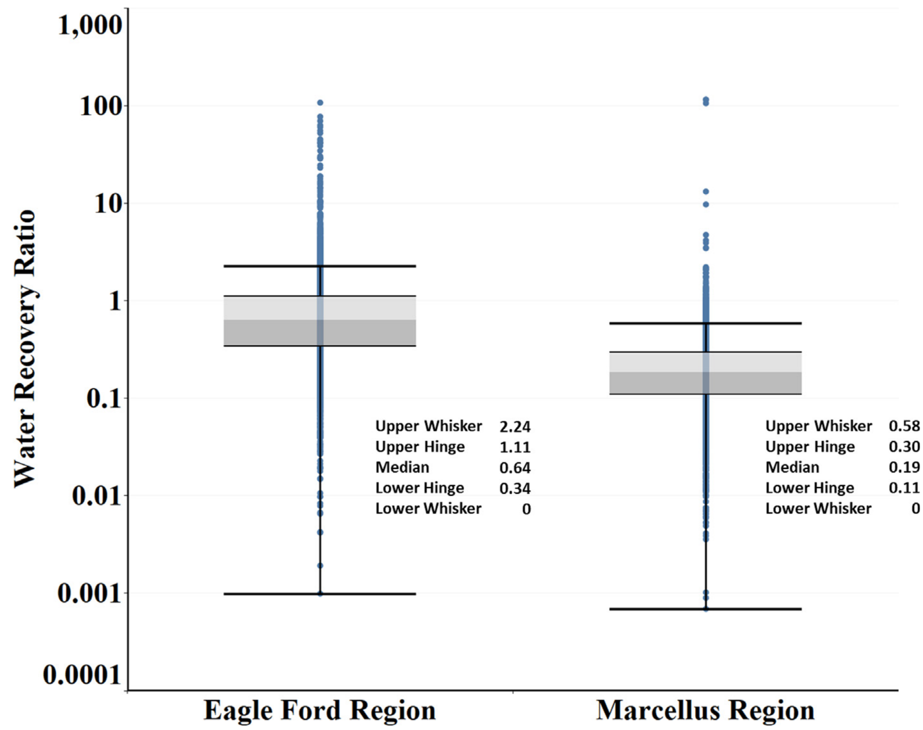


Fig. 6. Box plots of water recovery ratio data in the Eagle Ford region and Marcellus region.

whose values are less than 0.01 and the main reason should be the extremely small cumulative FP water production volume (Figs. 5(b) and 35(d)), which could be due to the reporting error or extremely short production history.

The box plots of the water recovery ratio data in the Eagle Ford and Marcellus regions are presented in Fig. 6, where the median, upper/lower whisker (i.e., the data within 1.5 times the interquartile range (IQR)) and upper/lower hinge (i.e., the 75th and 25th percentiles) value of each box plot are included. In these box plots, data points that lie outside the whiskers can be viewed as outliers, and thus they were discarded in this study before conducting the subsequent data analysis. Specifically, in the Eagle Ford region, the water recovery ratio data with the value greater than 2.24 were discarded; and in the Marcellus region, the water recovery ratio data with the value greater than 0.58 were discarded.

The main reason for the observed large variation in water recovery ratio within the same shale region is due to the significant difference in cumulative FP water production volume for a given water-use volume as presented in Fig. 7 (i.e., water-use volume is around 200,000 BBL). This is because the cumulative FP water production volume not only depends on the corresponding water-use volume but also the geological characteristics in the location where the well is drilled (e.g., porosity, permeability, water saturation).

It should be noted that the detailed information of geological characteristics is generally confidential, which makes the prediction of FP water production volume difficult and subsequent wastewater management inefficient. Thus, we used the water recovery ratio as a metric to evaluate the regional differences and then provided guidance for the development of efficient and sustainable water management strategies.

From this point of view, the collected water recovery ratio data were classified with respect to county, which are presented in Fig. 8. It shows that the water recovery ratios vary largely even within the same county. Since the data distribution in each county is highly right-skewed, we calculated the median value of water recovery ratio in each county to represent the generalized ratio value; due to this distributed nature in water recovery ratio within each county, the median value is more appropriate than the mean value to represent each county.

As shown in Fig. 9, the median water recovery ratios vary among the counties, which is due to the difference in geological characteristics over different counties, even though they are located within the same shale region.

To demonstrate how the different water recovery ratios may affect the design and configuration of SGSCN in the Marcellus region, the optimization model developed by Ahn et al. (2019) was adopted. As mentioned in Section 2.3, the water-use, FP water production and shale gas production volumes are the inputs to the SGSCN model, which were taken from the Marcellus well data. Based on Fig. 5(c) and (d), the water recovery ratios of around 75% of the collected wells in the Marcellus region are less than 0.3. Thus, in this study, we considered only the wells with the water recovery ratios around 0.1 and around 0.4 for Case 1 and Case 2, respectively. In both the case studies, three freshwater sources, three shale sites, three onsite treatment technologies (i.e., multistage flash (MSF), multi-effect distillation (MED) and reverse osmosis (RO)), three CWT facilities, five disposal wells, two processing plants, two underground reservoirs, and two power plants were considered. Note that the power plant is assumed to be the only monetization of the separated natural gas production and the generated electricity is directly sold to the market for profit. In particular, there are assumed to be maximum six potential wells that can be drilled in each shale site, all of which are assumed to have the same water and shale gas data. It is worthy to note that since the water-use volume is generally affected by technology development and economic considerations, which makes it more controllable than the water or gas production volumes, we chose the wells with similar water-use volumes (i.e., the different water recovery ratios are resulted from the different cumulative FP water production

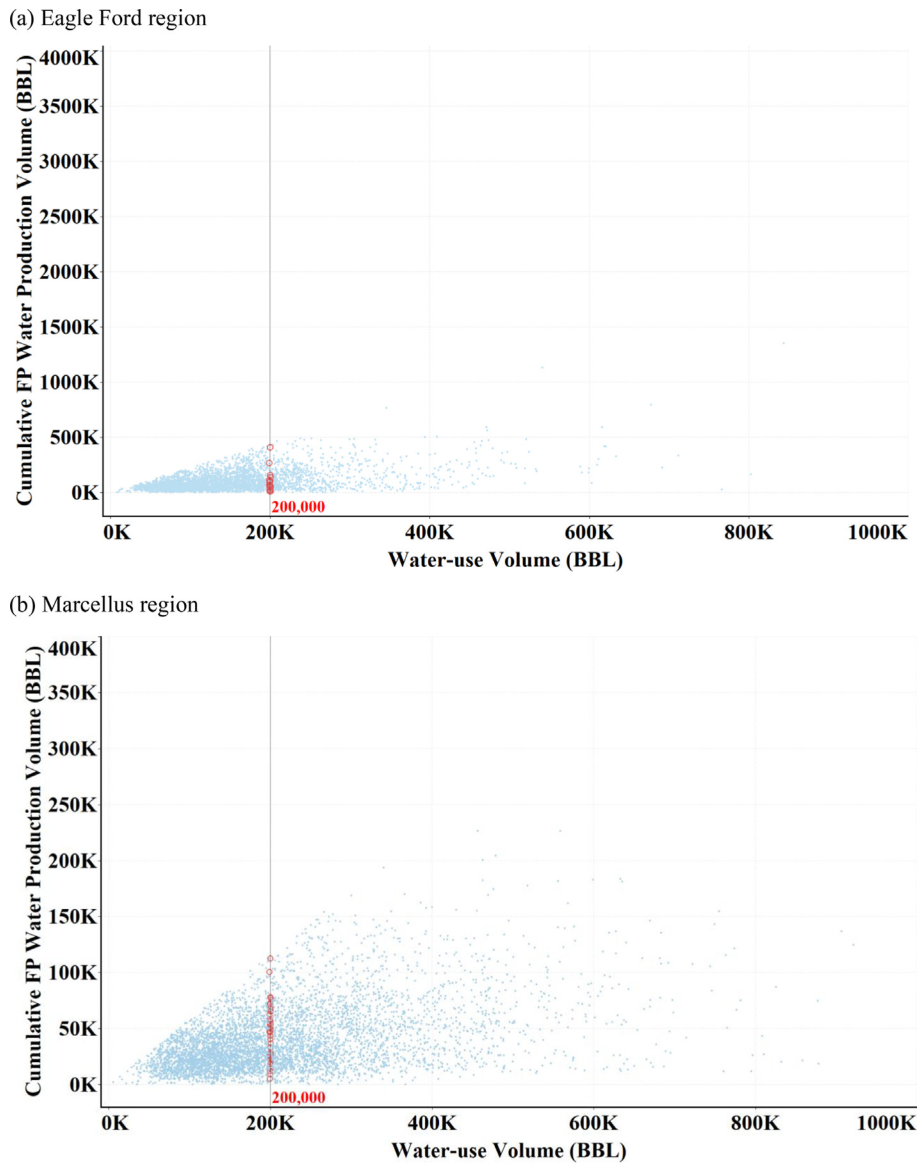


Fig. 7. Different cumulative FP water production volumes for a given water-use volume (around 200,000 BBL) in the (a) Eagle Ford region and (b) Marcellus region.

volumes). Thus, we considered three different levels of water-use volume to differentiate the three shale sites (i.e., 350,000 BBL in shale site 1, 250,000 BBL in shale site 2 and 150,000 BBL in shale site 3 in both the case studies). We also assumed that the compositions of methane and NGLs in shale gas are different in the three shale sites. Specifically, the volume fraction of methane is assumed to be 0.90, 0.85 and 0.80 in shale gas extracted from shale site 1, 2 and 3, respectively. Besides, since the FP water production data reported in the PA DEP database before 2015 are on a half-year basis and there are many missing monthly FP water production data in 2015, we considered the planning horizon as two years to obtain reliable input well data. The planning horizon is equal to the production period considered for each shale well and divided into eight quarters. The formulated SGSCN optimization model is a mixed-integer linear programming (MILP) model, which includes 2117 single variables, 343 discrete variables, and 2369 constraints. Implemented in the General Algebraic Modeling System (GAMS), the optimization model was solved using the solver CPLEX on a PC with Intel Core i7-6700 CPU @ 3.40 GHz and 16.00 GB RAM, running Windows 10, 64-bit operating system. After 3.343 and 1.875 CPUs of computational time, the optimal solutions for Case 1 and 2 were obtained with the global optimality gap of 0%, respectively.

The overall profit of the SGSCN is determined by the trade-off between the profits (from selling the NGLs and the generated electricity) and the costs (from freshwater acquisition, wastewater management, shale gas production and processing, storage, transportation and equipment). As presented in Fig. 10(a), to maximize the overall profit in Case 1 (i.e., water recovery ratio as 0.1), one well in shale site 1 and five wells in shale site 2 are drilled using the freshwater transported from freshwater source 2 by pipeline. To treat the generated FP water, only CWT facility 1 is required; to handle the produced shale gas, processing plant 1 is needed for the separation of shale gas while two power plants are used to generate the electricity with the obtained natural gas production. Underground reservoir 1 is also required to storage some natural gas before being sent to power plant 1. By comparison, in Case 2 (i.e., water recovery ratio as 0.4) as presented in Fig. 10(b), three wells in shale site 1 and one well in shale site 3 are drilled. Further, all the FP water generated in shale site 1 is injected to disposal well 1 while the FP water in shale site 3 is treated by onsite treatment facility

(a) Eagle Ford region

Water Recovery Ratio	Bee	DeWitt	Dimmit	Frio	Gonzales	Karnes	La Salle	Lavaca	Live Oak	Maverick	McMullen	Webb
0.0		22	68			17	24		9		1	15
0.1		59	89	1		55	30		25		12	64
0.2	1	68	82			79	24	1	42	3	21	59
0.3	1	54	85			86	27		33		23	88
0.4	1	42	91			67	33	1	23	2	27	105
0.5	2	19	93			46	29		17	1	18	122
0.6		10	69			34	23	1	17	1	9	106
0.7		6	75			27	18		6	1	13	139
0.8	1	3	68			27	11		7	1	11	114
0.9	2	4	39			22	17		6		9	86
1.0		4	33	1	1	13	13		9		3	76
1.1		2	34			19	7		6		5	78
1.2		1	30	1		12	8		2		5	59
1.3			22	1		10	12		5		4	54
1.4		1	15			10	7		5		2	31
1.5			13	1		14	2		3		1	34
1.6			13			9	5		2		2	24
1.7		1	14	1		9	8		4			29
1.8		1	8			6	2		4			10
1.9	1		11			14	6		3		1	14
2.0		2	6			3	3		1			9
2.1			4	1		6	6		1			11
2.2			1			3	1					4

(b) Marcellus region

Water Recovery Ratio	Allegheny	Armstrong	Beaver	Bradford	Butler	Cameron	Centre	Clarion	Clearfield	Clinton	Crawford	Elk	Fayette	Forest	Greene	Huntingdon
0.00		11	14	47	15	2	1			4		4	6	1	18	
0.05	15	8	14	87	86	2			4	1		4	12		61	
0.10	10	24	14	113	110	5	1	1		2		2	9		94	
0.15	10	11	11	111	97		2	1	1	2		10	8		107	
0.20	17	7	6	72	52				3	1		6	3	1	109	
0.25	4	5	6	47	22	2	1		1	3		5	11		86	
0.30	8	4	1	24	11	2		1	2	6		17	9		72	
0.35	9	2		11	3	4				4		17	6	2	44	
0.40	4		4	5	1	4		2				12	5		33	
0.45	2			5	3	8			2	1		10	7	1	21	
0.50	2				1	7		1	1	1	1	7	5	1	21	1
0.55	1					6						6	6		6	

Water Recovery Ratio	Indiana	Jefferson	Lawrence	Lycoming	McKean	Mercer	Potter	Somerset	Sullivan	Susquehanna	Tioga	Venango	Warren	Washington	Westmoreland	Wyoming
0.00	2		1	18	3	1			5	133	16			29	2	33
0.05	2		8	37	1	6	2		39	248	48			133	5	67
0.10			24	76		6	2	4	30	255	45	1		123	12	38
0.15		3	5	77	1	6		2	15	178	61			126	10	14
0.20	2	1	2	64	1	11	4	2	5	106	57			149	7	17
0.25		3	4	74	3	10	4		4	52	42			97	9	19
0.30	1	3	3	60	1	6	6	1	1	27	42		1	80	8	3
0.35	1		2	35	4	2	5		1	20	29	1		48	12	2
0.40	1	5	2	26	8	2	5		2	11	21	1		21	6	
0.45	1	2	1	24	8		2			9	17			19	7	
0.50	1			13	11		4			4	10			9	2	3
0.55		1		8	4		2			4	5			4	3	

Fig. 8. Histograms of the water recovery ratio data in each county in the (a) Eagle Ford region and (b) Marcellus region.

using MSF. As presented in Fig. 11, the overall profits in the two case studies are close (i.e., the difference is around 1%). However, in Case 1, the total freshwater cost is 54% higher than the one in Case 2 while the associated total wastewater management cost is 59% lower, which indicates significantly different optimal configurations of water network.

Since the number of drilled wells in Case 1 is relatively more than the one in Case 2, the resulting total amount of freshwater in the former is larger than the latter as shown in Table 1; the associated freshwater costs are presented in Fig. 11. To obtain the large amounts of freshwater as required in both the case studies, freshwater source 2 is generally used due to the larger capacity than freshwater source 1, as well as the shorter distance to the shale sites than freshwater source 3. Note that since the maximum capacity of a truck is 135,000 BBL, pipeline is always the only feasible transportation mode. On the other hand, as indicated by the high water recovery ratio in Case 2, the total amount of generated FP water (i.e., 360,465 BBL) is even larger than the one (i.e., 97,452 BBL) in Case 1. Thus, comparing to using the CWT facility as Case 1, it is more economically preferred to directly inject the FP water to the disposal well in Case 2 regardless of the long distances between the shale sites and disposal wells. As for shale site 3 in Case 2, since the shale well is drilled at the end of the planning horizon and thus only the FP water production within the first quarter of its production period is considered, the onsite treatment facility is chosen to avoid the high transportation cost and save some freshwater cost by reusing the treated water for other hydraulic fracturing jobs. Even though the recovery factor (i.e., the ratio of recycled water volume to FP water volume) of MSF is the lowest and the associated unit treatment cost is the highest among the three available technologies, it is the only feasible choice since the capacities of the other two (i.e., MED and RO) are not enough to handle the FP water from shale site 3. It is worthy to note that even with the mentioned benefits from onsite facility treatment, it is still almost the last choice in both the case studies, due to its much higher unit treatment cost than the ones associated with the CWT facilities and disposal wells as well as the fact that reused water is not required in many planning periods. As a result, the total wastewater management cost in Case 2 becomes much higher than the one in Case 1.

Unlike the FP water production, the total amount of shale gas production in Case 1 (i.e., 10,436,245 mcf) is similar to the one in Case 2 (i.e., 10,748,967 mcf). However, since the shale gas production cost also contains the drilling and hydraulic fracturing costs which are dependent on the number of drilled wells in the shale sites, the resulting shale gas production cost in Case 1 is 10% higher than the one in Case 2. On the contrary, the shale gas processing plant cost (i.e., including capital cost of processing plant, operating cost of processing plant and transportation cost of shale gas between shale sites and processing plants) only depends on the amount of shale gas production, thus it is reasonable to observe that the shale gas processing plant cost in Case 2 is higher than the one in Case 1. Besides, since a large proportion of the shale gas production in Case 2 is generated from shale site 1 (i.e., 10,370,898 mcf from shale site 1 and 378,069 mcf from shale site 3) where the composition of NGLs is the smallest among the three shale sites, the total amount of NGLs production in Case study 2 is found to be relatively less than those in Case 1 while the total amount of natural gas production is still more. Thus, the associated profit from selling the NGLs is less than the one in Case 1 while the profit from selling the electricity, electricity generation cost and total transportation cost between processing plant and power plant are higher. In both the case studies, processing plant 1 is chosen due to its shorter distance to the following underground reservoirs and power plants. Further, even though both the power plants are always needed to maximize the overall profit, one processing plant is enough to handle all the shale gas production to meet electricity demand. Note that underground reservoir 1 is necessary to temporarily store those natural gas which cannot be transported to the power plants immediately.

Based on the cost breakdowns shown in Fig. 12, the economic performance of the water network is almost negligible in comparison to the shale gas network in the two case studies. Thus, it should be generally preferred to drill more wells and schedule them to be completed as early as possible to obtain more shale gas production for maximized overall profit. Based on the optimal solutions presented in Table 1, in Case 1, the amount of NGLs sold as well as the natural gas transported for electricity generation always reaches the maximum demand except the first quarter. To obtain more production in the first quarter, the first well is drilled in shale site 1 where the shale gas production is greater than the other two shale sites. Similar phenomenon can be observed in Case 2. In particular, drilling the well in shale site 3 at the end of the planning horizon is necessary since the NGLs and natural gas production in the eighth quarter from the wells drilled in shale site 1 are not enough to achieve the maximum products demands simultaneously. Thus, it is the provided maximum NGLs demand as well as the maximum natural gas demand that limits the number of wells to be drilled and determines the sequence and timing of the hydraulic fracturing jobs. From this point of view, the different schedules applied in the two case studies should be mainly the result of different shale gas production profiles of the wells considered. On the other hand, even though the total shale gas production may be managed to be close to the maximum demand for the overall economic performance, the total FP water production volume can be largely different, which is indicated by the different water recovery ratios in different regions as presented in Fig. 9(b). The two case studies suggest that when the water recovery ratio is low, the amount of FP water production is small and thus CWT or onsite treatment facility are generally economically and environmentally preferred; however, when the water recovery ratio is high, the amount of FP water production is large and thus disposal well is generally the first choice due to the much lower injection cost than the treatment costs in CWT and onsite treatment facilities. Note that the availability of these units and the associated transportation costs are also the important determinants. Thus, even though the final objective is the same (i.e., to achieve the maximized overall profit), the designs and configurations of SGSCN can be significantly different in different regions, especially the optimal water network.

REMARK. There are two primary novel contributions of this work in the areas of methodologies and with respect to results. The proposed methodology is the first systematic approach to integrate the spatial and temporal variabilities in FP water with the management strategies. From the perspective of results, this work has definitively provided a response to the critical question of whether the recover ratio for shale gas water over a time horizon is > 1 or <1. Various inconsistent results and observations have been reported in the literature. In this work, we have used numerous field data and applied state-of-the-art data analytics to generate an objective answer which is crucial for water management strategies because it leads to fundamentally different approaches (e.g., reuse versus treatment and discharge). The following is more explanation of the novel contributions. The efficient management of freshwater and

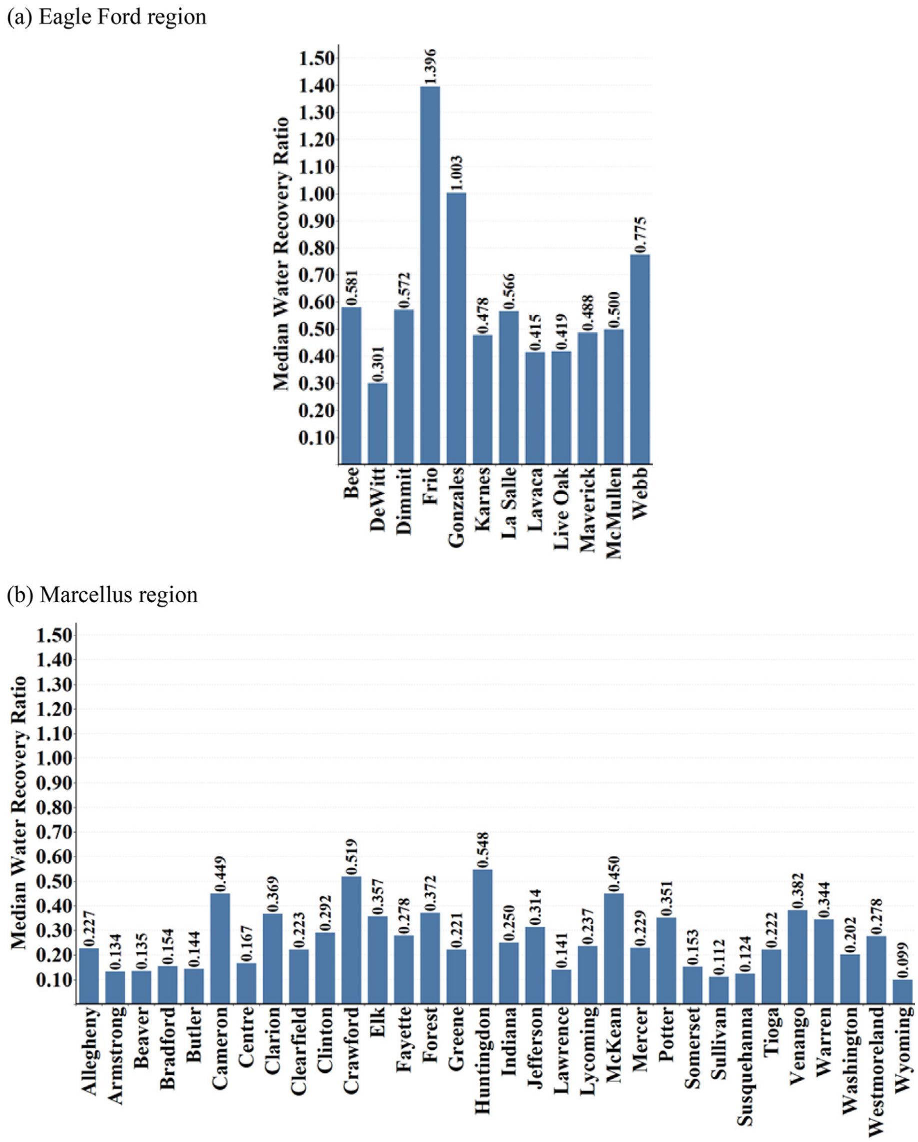


Fig. 9. Median water recovery ratio in each county in the (a) Eagle Ford region and (b) Marcellus region.

FP water is of vital importance to sustainable development of the shale gas industry, especially in water-scarce regions. In this regard, we collected water-use and FP water volume data from several databases and conducted systematic data analyses. In this study, we mainly focused on the water recovery ratio, instead of the two water volumes. Since the water recovery ratio is determined by interplay between geological characteristics of each well and the amount of injected fracturing fluid, it can provide a unique understanding of each well. Specifically, for a given volume of hydraulic fracturing fluid to be injected, the water recovery ratio can provide a unique predictive power of the corresponding FP water volume. Compared with a traditional approach of utilizing historical FP water data, it is more reliable since it can readily take into account a change in water-use volume (i.e., due to change in fracturing technology or shale development strategy) for accurate prediction of FP water volume. Furthermore, well-to-well variability due to spatial heterogeneity in geological characteristics can be directly considered in the presented data analysis through the spatial analysis of water recovery ratio over multiple counties in Marcellus and Eagle Ford regions. This spatial variation in water recovery ratio can serve as a reference for selection of locations and capacities of treatment facilities. The fundamental understanding of spatial variation in water recovery ratio and how it may affect the optimal design and configuration of SGSCN can also help design the shale gas system in a distributed manner for regional-scale water management as well as effective coordination of local and national level of water management, which could be the key to sustainable development of the shale gas industry.

4. Conclusions

In this study, we focused on presenting and analyzing the water recovery ratios of the shale gas wells drilled in the Eagle Ford and Marcellus shale regions, by utilizing the integrated water-use and FP water production volume data collected from multiple database sources. The overall objective is to use the water recovery ratio as a

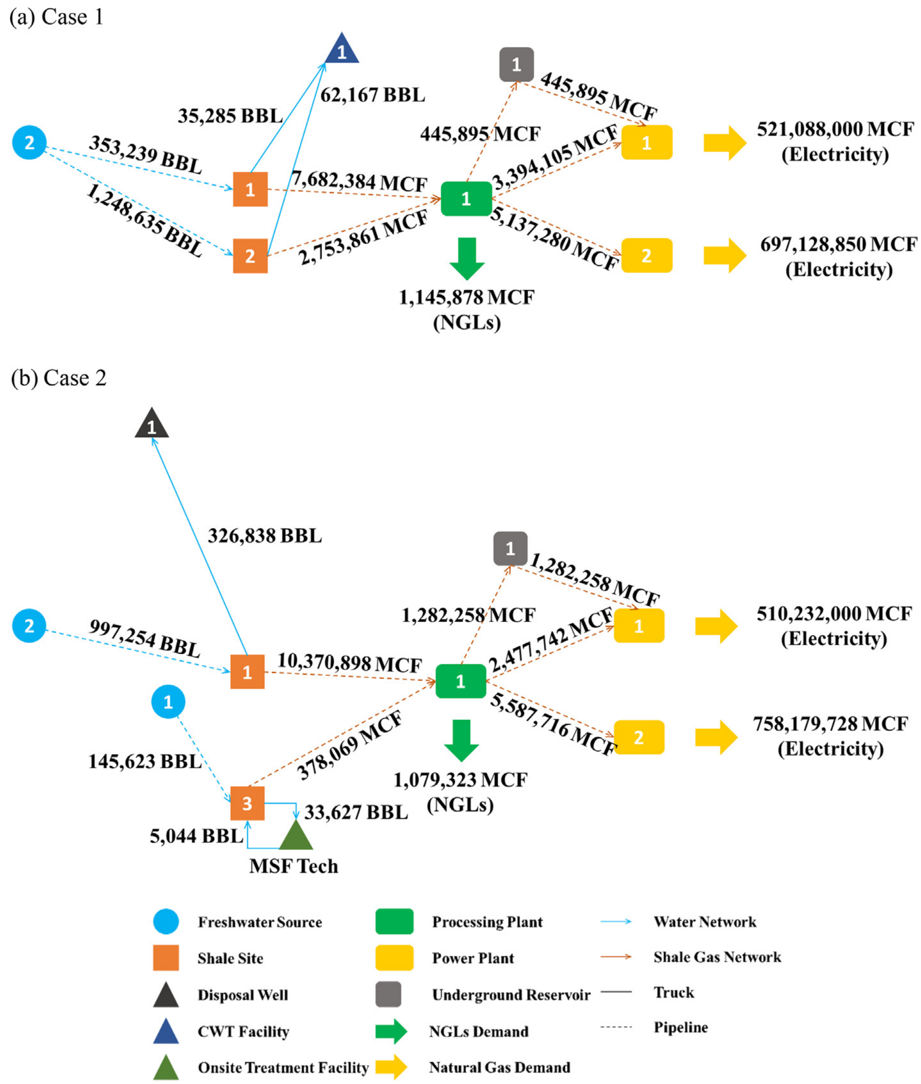


Fig. 10. Comparison of optimal SGSCN configurations in (a) Case 1 and (b) Case 2.

metric to characterize the shale gas wells, so as to provide guidance for the design and configuration of SGSCN in shale gas development. Based on the obtained data, in the Eagle Ford region, 30% of the collected wells had the water recovery ratio greater than 1; however, in the Marcellus shale region, only 1% of the collected wells had the water recovery ratio greater than 1 while 75% of the collected wells had the water recovery ratio less than 0.3. Besides the large discrepancy in water recovery ratio between the two shale regions, the water recovery ratios also varied across multiple counties in each shale region. Specifically, by calculating the median water recovery ratio in each county, the median value ranged from 0.3 to 1.4 and from 0.1 to 0.5 in the Eagle Ford region and Marcellus region, respectively. Then, two case studies were presented, where two groups of wells with similar water-use volumes but different water recovery ratios were considered. When the water recovery ratio was low, the generated FP water was transported to nearby CWT facilities for treatment before being safely discharged to surface water; on the other hand, when the water recovery ratio was high, it was economically preferred to directly inject the FP water to disposal wells. Treatment using advanced technology in onsite facilities for reuse was considered only when the FP water production volume was small and there existed water demands. Thus, the water recovery ratio of shale gas well can decisively determine which water management strategy is the most profitable choice, and thus different SGSCN configurations should be considered for the wells with different water recovery ratios.

CRediT authorship contribution statement

Kaiyu Cao: Conceptualization, Methodology, Validation, Formal analysis, Investigation, Writing - original draft, Writing - review & editing, Visualization. **Prashanth Siddhamshetty:** Validation, Formal analysis, Investigation, Writing - review & editing, Visualization. **Yuchan Ahn:** Methodology, Validation, Formal analysis, Investigation. **Mahmoud M. El-Halwagi:** Conceptualization, Writing - review & editing, Supervision, Project administration, Funding acquisition. **Joseph Sang-Il Kwon:** Conceptualization, Formal analysis, Resources, Writing - review & editing, Supervision, Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

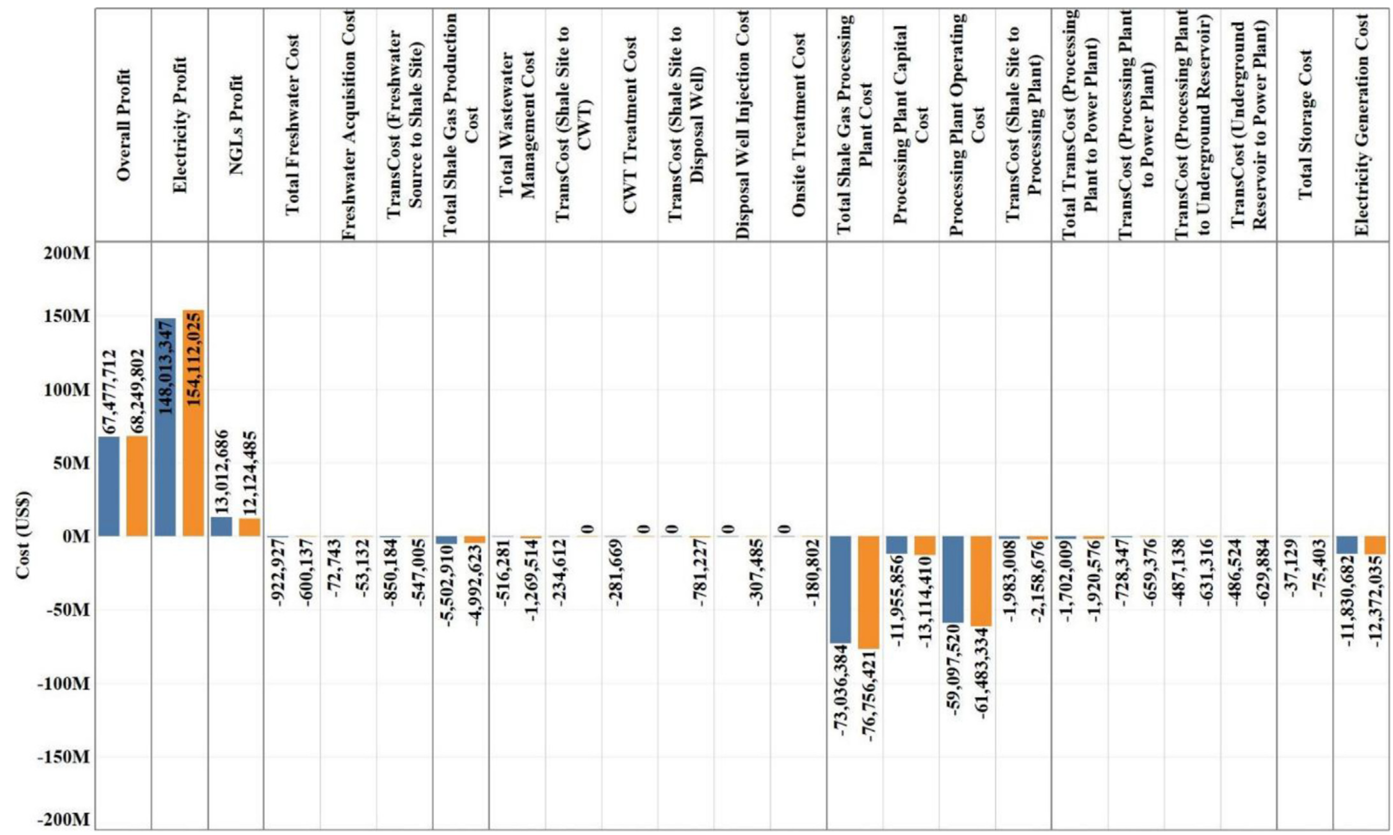


Fig. 11. Comparison of the detailed costs in the two case studies (Case 1 is represented by blue; Case 2 is represented by orange). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Table 1
Comparison of freshwater acquisition, NGLs and natural gas production in the two case studies. (a) Case 1 (water recovery ratio = 0.1). (b) Case 2 (water recovery ratio = 0.4).

		T1	T2	T3	T4	T5	T6	T7	T8
Hydraulic Fracturing Operations	Availability	2	2	2	2	2	2	2	2
	Optimal	1*	1	–	–	2	1	1	–
Freshwater Source 1 (BBL)	Availability	150,000	150,000	150,000	150,000	150,000	150,000	150,000	150,000
	Optimal	–	–	–	–	–	–	–	–
Freshwater Source 2 (BBL)	Availability	3,075,000	3,075,000	3,075,000	3,075,000	3,075,000	3,075,000	3,075,000	3,075,000
	Optimal	353,239	249,727	–	–	499,454	249,727	249,727	–
Processing Plant 1 (NGLs, MCF)	Max Demand	120,000	128,571	137,143	145,714	154,286	162,857	171,429	180,000
	Optimal	65,878	128,571	137,143	145,714	154,286	162,857	171,429	180,000
Power Plant 1 (Natural Gas, MCF)	Max Demand	480,000	480,000	480,000	480,000	480,000	480,000	480,000	480,000
	Optimal	480,000	480,000	480,000	480,000	480,000	480,000	480,000	480,000
Power Plant 2 (Natural Gas, MCF)	Max Demand	720,000	720,000	720,000	720,000	720,000	720,000	720,000	720,000
	Optimal	97,280	720,000	720,000	720,000	720,000	720,000	720,000	720,000
Hydraulic Fracturing Operations	Availability	2	2	2	2	2	2	2	2
	Optimal	2	1	–	–	–	–	–	1*
Freshwater Source 1 (BBL)	Availability	150,000	150,000	150,000	150,000	150,000	150,000	150,000	150,000
	Optimal	–	–	–	–	–	–	–	145,623
Freshwater Source 2 (BBL)	Availability	3,075,000	3,075,000	3,075,000	3,075,000	3,075,000	3,075,000	3,075,000	3,075,000
	Optimal	664,836	332,418	–	–	–	–	–	–
Processing Plant 1 (NGLs, MCF)	Max Demand	120,000	128,571	137,143	145,714	154,286	162,857	171,429	180,000
	Optimal	119,037	128,571	137,143	145,714	125,027	98,011	145,819	180,000
Power Plant 1 (Natural Gas, MCF)	Max Demand	480,000	480,000	480,000	480,000	480,000	480,000	480,000	480,000
	Optimal	400,000	480,000	480,000	480,000	480,000	480,000	480,000	480,000
Power Plant 2 (Natural Gas, MCF)	Max Demand	720,000	720,000	720,000	720,000	720,000	720,000	720,000	720,000
	Optimal	547,176	720,000	720,000	720,000	720,000	720,000	720,000	720,000

*Note that the well in T1 is drilled in shale site 1; the other wells are drilled in shale site 2.
*Note that the well in T8 is drilled in shale site 3; the other wells are drilled in shale site 1.

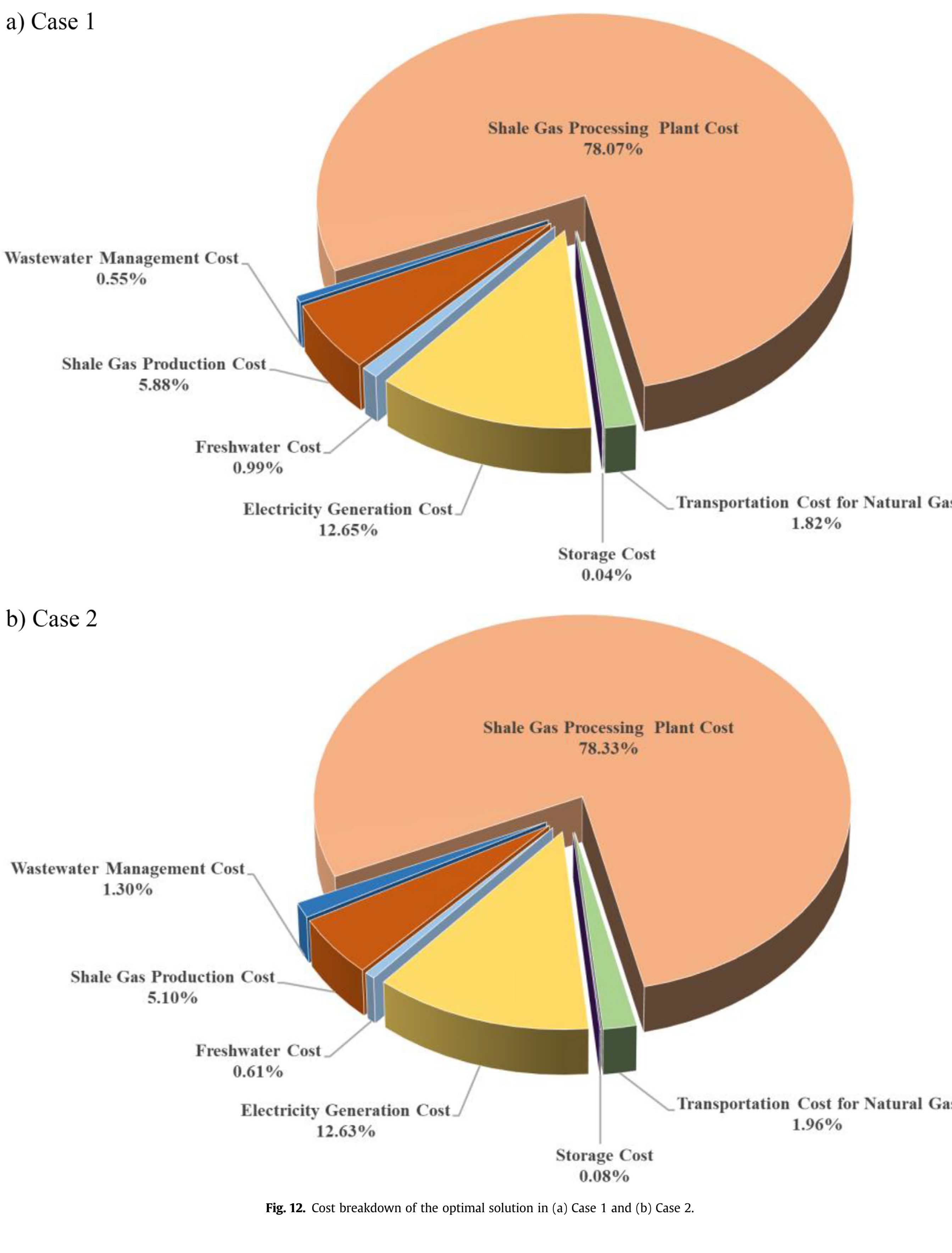


Fig. 12. Cost breakdown of the optimal solution in (a) Case 1 and (b) Case 2.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2020.123171.

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