Chapter 2
Shale Gas Process and Supply Chain Optimization

Jiyao Gao, Chang He and Fengqi You

Abstract In recent decades, large-scale production of shale gas has been considered as a major issue in the U.S. energy industry. In accordance with its great economic potential and environmental concerns, shale gas process and supply chain optimization has become one of the most popular research areas. In this chapter, we provide a comprehensive overview of the supply chain management and process design problems in shale gas industry. We summarize four major research challenge areas, namely the design and planning of shale gas supply chain, water management in hydraulic fracturing, sustainability concerns in shale gas industry, and design and optimization in shale gas processing system. We further provide review and discussions of the major publications corresponding to each of the aforementioned topics. Potential opportunities in the shale gas system are presented as well to illuminate the future research.

2.1 Introduction

Shale gas is known as unconventional natural gas extracted from shale rock layer and has emerged as one of the most promising energy sources within the last few decades. With the discovery of huge shale gas reserves all over the world, a "shale revolution" starts in the U.S. and keeps spreading out in other countries. In 2005, the U.S. barely produces any natural gas from shale formations. Nowadays, nearly 44 % of the total natural gas withdrawal is from shale gas wells (EIA 2011).

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According to the Annual Energy Outlook 2015 by the U.S. Energy Information Administration (EIA 2015), natural gas production is expected to grow by an average rate of 1.6 % per year from 2012 to 2040. As a result, the percentage of the U.S. total natural gas production from shale gas is expected to increase to 53 % by 2040.

The remarkable development of large-scale shale gas production would not be possible without the hydraulic fracturing and horizontal drilling technologies (Gregory et al. 2011; Vengosh et al. 2013). Different from the conventional natural gas, shale gas is embedded in the shale rocks that can be a few thousand feet deep. Therefore, special techniques are required to withdraw this unconventional resource. By using hydraulic fracturing, millions of gallons of fracturing fluid (about 90 % water, 9.5 % sand, and 0.5 % chemical additives) is pumped underground under high pressure (up to 70 Mpa), fracturing the rock layer and holding fractures open, thus forcing the shale gas and/or oil to flow back to the surface. The horizontal drilling, on the other hand, is a drilling process in which the well is turned horizontally at depth. Compared with the vertical drilling, horizontal drilling allows us to drill multiple wells at a single shale site/pad. As a result, a horizontal well site is able to produce more energy with fewer wellbores, which significantly reduces the capital investment and improves the efficiency for shale gas production (Hughes 2013).

Shale gas production of a single well normally features a high initial production rate followed by an astounding decline from 60 to 90 % after the first three years (Hughes 2014). This characteristic is mainly caused by the pressure depletion and inherently low permeability of the reservoir. Consequently, operators need to regularly drill new wells to maintain a stable production profile, which results in a scheduling problem. Additionally, based on the composition, shale gas can be classified as dry gas and wet gas, and the key difference is the content of natural gas liquids (NGLs). The NGLs are defined as light hydrocarbons including ethane, propane, butane and heavier components, which typically have substantially higher market values than methane gas. Dry gas is almost pure methane with trace NGLs. Although methane is still the dominant component in wet gas, the amount of NGLs is significant enough to require further processing. Depending on the location, both the estimated ultimate recovery (EUR) and shale gas composition of a shale well may have significant variance. All of these issues render the optimal design and operation in the shale gas industry a challenging topic.

Apart from the shale gas itself, the wide application of hydraulic fracturing has resulted in another serious issue, known as the shale water management problem (Nicot and Scanlon 2012; Mauter et al. 2013, 2014; Small et al. 2014; Yang et al. 2014; Mauter and Palmer 2014). The hydraulic fracturing operation during the shale gas production process requires a massive amount of freshwater (Jiang et al. 2014). Till 2012, a total of 63,000 shale wells have been reported in the U.S., and each well requires approximately 4–6 million gallons of water for fracturing and production (EPA 2011; API 2010; Paper 2008; Nicot et al. 2014). Such a huge consumption of fresh water resource can cause severe consequences on local water supply especially in water-scarce territories. Moreover, during hydraulic fracturing process, a large portion of injected fluid flows back to the surface as highly contaminated wastewater, which contains high concentration of total dissolved solids (TDS) as well as other toxic and radioactive dissolved constituents (Soeder and Kappel 2009; Rahm and Riha 2012). Due to the increasing public concern on the water related environmental issues, it is imperative to develop an effective approach to address challenges in the shale water management problem.

The shale gas produced at shale site is generally considered as raw shale gas that needs further processing. The processing service is typically provided by midstream processors. Through the shale gas processing, impurities such as compounds and gases, oil, and water mixed with the natural gas are removed. Two major products, "pipeline-quality" sales gas and NGLs, are extracted and sold separately. The sales gas is normally delivered to major intrastate and interstate pipeline transmission systems and further sent to final customers. The NGLs, on the other hand, can be used as feedstock for the production of value-added chemicals, such as olefins and gasoline blending stocks. With the rapid development of shale gas industry, excessive supply of NGLs requires more cost-effective shale gas processing designs and conversion alternatives for a better use of this valuable byproduct (He and You 2014; Ehlinger et al. 2014).

Despite the great economic potential stimulated by the shale gas, one major concern impeding the expansion of shale gas industry is its negative impact on the climate change. Methane is about 25 times more potent greenhouse gas (GHG) than carbon dioxide based on the 100-year global warming potential (GWP). A small amount of methane leakage could lead to enormous greenhouse gas footprint (Howarth 2014). Additionally, supply chain activities such as shale gas production, processing, transportation, and gas-based power generation could incur large amount of GHG emissions as well (Allen 2014a, b; Zavala-Araiza et al. 2015). There have been extensive studies published evaluating the life cycle carbon footprint of shale gas (Jiang et al. 2014; Harto 2013; Dale et al. 2013; Burnham et al. 2011; Stephenson et al. 2011; DOE/NETL 2011; Laurenzi and Jersey 2013; Alvarez et al. 2012; Brandt et al. 2014). However, the shortage of decision-support tools and methodologies still exists, which requires the development of corresponding optimization models for more sustainable design alternatives in the shale gas industry.

This chapter reviews the most recent advances in application of mathematical programming techniques for optimization of shale gas process and supply chain designs. The remaining content of this chapter is organized as follows. We first present a comprehensive review of recent literature on strategic design and planning of shale gas supply chain. Next, we introduce the water management problem in the shale gas system and explore the application of life cycle optimization approach in the shale gas supply chain. After that, we focus on the shale gas processing and conversion alternatives from a process design perspective. Finally, we present challenges and opportunities for future shale gas development and conclude the chapter.

2.2 Design and Planning of Shale Gas Supply Chain and Water Management

2.2.1 Shale Gas Supply Chain Network

The shale gas supply chain is a complex system involving shale gas suppliers in the upstream, shale gas processors in the midstream, and distributors in the downstream (Chima 2011; Seydor et al. 2012). In this section, we provide a comprehensive overview of a typical shale gas supply chain structure and corresponding design decisions. The major stages of a shale gas supply chain are summarized in the following Fig. 2.1.

2.2.1.1 Shale Site Construction

First, potential shale wells are explored through geologic evaluation. Once a potential shale site is identified, the well operator needs to reach a lease agreement with the corresponding landowner and then obtain the drilling permits. It is the operator's responsibility to guarantee that all the following drilling and production activities will be carried out in accordance with relevant regulations. After the approval of the operator's permit by local environmental regulation agencies, the site construction and well drilling can start.

The shale site is typically constructed following these steps: the first step involves the clearance of proposed area and the accommodation of equipment. Meanwhile, a road way is constructed to provide access to the shale site. Subsequently, pits/impoundments are constructed to properly handle the fluids during drilling and hydraulic fracturing. Next, pipelines associated with shale sites are installed, including gathering lines, injection lines, and water supply lines. Other infrastructures such as storage tanks are built as well.

2.2.1.2 Drilling, Fracturing, and Production

After the shale site construction, the drilling rig is moved on site and assembled. A conductor hole is predrilled, and then conductor pipes are inserted to prevent soft rocks from caving and conduct drilling mud from bottom to the surface during drilling process. Depending on the number, depth, and length of horizontal wells to

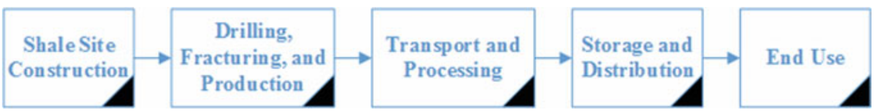

Fig. 2.1 Overview of shale gas supply chain

be drilled, the drilling stage can last for a few months, which requires a constant supply of drilling fluid and proper handling of sediments and wastewater. Once the drilling is completed, protective casing and cementing are used.

The following stage is the well completion, which mainly involves the hydraulic fracturing operation. A mixture of water, sand, and chemical additives is injected underground at a high pressure to break up shale-rock formations, such that fractures are created and held open by proppant, and then shale gas and oil can be extracted. Typically, the horizontal wells are stimulated by stages, depending the specific fracturing schedule and technology applied, the hydraulic fracturing stage could last for several months. Once fracturing is completed, a wellhead is constructed, and the local gathering pipelines are prepared for the controlled extraction of natural gas.

2.2.1.3 Transport and Processing

The transportation of shale gas is mainly carried out by pipelines. The pipeline system includes all the equipment such as pumps, valves, meters, and monitoring devices. After shale gas is produced, water and condensate are typically removed at or near wellhead. Then, gathering lines (6–20-in. diameter) are used to take the raw shale gas to processing facilities, where sales gas that meets the pipeline specifications and valuable NGL products are obtained. Gathering lines are typically considered as the demarcation between upstream production and midstream processing and transmission to market.

The shale gas processing plant is a dedicated separation train that consists of a series of processes, including gas sweetening, dehydration, NGL recovery, and N_2 rejection. If economically feasible, NGLs may be further separated into ethane, propane, butanes, and pentanes+streams in a NGLs fractionation train. Notably, for dry gas that is almost pure methane, processing might be unnecessary (Cafaro and Grossmann 2014). As a result of the rapid development of shale gas industry, expansion of infrastructure including pipelines and processing plants is getting necessary, and the high capital investment of these infrastructures requires an optimal strategy for the corresponding design decisions.

2.2.1.4 Storage and Distribution

Like other commodities, the produced shale gas can either be directly transported to interstate/intrastate pipeline system for distribution or transported to underground reservoirs and stored for an indefinite period of time. There are three principle types of underground storage sites in the U.S. today, including the depleted natural gas or oil fields, aquifers, and salt caverns (EIA Underground Natural Gas Storage 2014). The underground reservoirs can behave as a “buffer” in the shale gas supply chain to accommodate fluctuations in natural gas demand and price.

The distribution system is in charge of delivering the shale gas to end-use customers. While large customers such as power plants may receive gas directly from the interstate or intrastate pipelines, most individual customers buy gas from distribution companies. The transmission cost could account for up to half of the total distribution cost, in addition to the commodity cost. Depending on the specific function, the transmission pipeline can be 6–48 in. in diameter. As a result, the corresponding capital investment of these pipelines can be significantly different. Thus, it is important to design proper capacity for the distribution pipeline system.

2.2.1.5 End Use

Natural gas is priced and traded as a commodity at different locations throughout the country. These locations are known as market hubs that are normally located at the intersection of major pipeline systems. The biggest market hub is Henry Hub located in Louisiana, and the spot and future natural gas prices set at Henry Hub are generally considered as the primary price set for the North American natural gas market. Depending on the specific usage, the natural gas consumption can be classified into three major partitions, including lease and plant fuel, pipeline and distribution use, and volumes delivered to consumers. There are four types of end-customers, namely power plants, industrial customers, commercial customers, and residential customers (EIA Natural Gas Consumption by End Use 2015).

2.2.2 Optimization Models for Shale Gas Supply Chain

Conventional natural gas supply chain has been fully studied in the literature. A variety of models have been proposed addressing the design and planning problems in oil/gas supply chains (Duran and Grossmann 1986; Iyer et al. 1998; van den Heever and Grossmann 2000; Gupta and Grossmann 2012). In recent decades, with the rapid development of shale gas industry, many research studies arise specifically focusing on the optimization of shale gas system. Knudsen and Foss (2013) present a novel operational scheme for enhanced utilization of late-life shale gas systems. In this work, a large number of geographically distributed wells and pads are considered, which are producing at low erratic rates due to reservoir pressure depletion and well liquid loading. By using a shale-gas well and reservoir proxy model, a generalized disjunctive program (GDP) is formulated. The proposed cyclic shut-in and production strategy is expected to avoid well liquid loading and improve the overall production. Following this work, Knudsen et al. (2014) propose a Lagrangian relaxation-based decomposition scheme for solving large field-wide well scheduling problems in shale gas systems. Furthermore, they explore the integration of shale gas supply with local natural-gas power generation. A large-scale mixed-integer linear program (MILP) is proposed, and the results indicate a potential increase of profit for shale gas operators by improving well scheduling (Knudsen et al. 2014).

The first mathematical model addressing the long-term strategic planning and design of the shale gas supply chain is proposed by Cafaro and Grossmann (2014). The authors propose a large-scale nonconvex mixed-integer nonlinear program (MINLP) model to determine the optimal design of shale gas supply chain. Critical decisions, including the drilling and fracturing plan, the location and sizing of processing plants, the length and location of gas and liquid pipelines, and the power of gas compressors, are simultaneously addressed. The overall objective is defined as maximizing the net present value (NPV) of the project over a 10-year planning horizon. Features such as decreasing production rate of shale wells, variant shale gas composition, and concave cost functions for capital investment are captured. A real-world case study based on Marcellus shale play is considered and solved by a tailored branch-and-refine-optimization approach. From the results of this work, the importance of NGLs to the economics of the project is identified especially considering the low natural gas price. In addition, the optimal drilling and fracturing scheduling could maximize the utilization of processing and transportation infrastructure, thus significantly improving the overall economics and energy/resource efficiency.

In spite of the optimistic forecast of shale gas development, a recent report unveils the fact that the actual profitability of a shale well can be significantly affected by various uncertainties, especially uncertainty of EUR (Hughes 2014). There are some studies evaluating the influence of uncertainty in shale gas supply chain based on general analysis and numerical models (Gracceva and Zeniewski 2013; Jayakumar and Rai 2012; Chaudhri 2012; Harding 2008). However, few of them provide a systematic approach to tackle the shale gas supply chain optimization problem under uncertainty.

Identifying such a knowledge gap in the shale gas supply chain literature, Gao and You (2015) present a comprehensive shale gas supply chain model that not only considers design and planning decisions, but also properly addresses EUR uncertainty of shale wells. In this work, a shale gas supply chain covering the upstream producers to the downstream end-customers is considered, as shown in Fig. 2.2. The EUR distribution is derived from real data reported in literature (EIA 2011; Swindell 2014). By reviewing the distribution of EUR, a distinct "long tail" is observed. Thus, a scenario-based stochastic programming approach is adopted as the suitable method accounting for EUR uncertainty. The resulting problem is formulated as a two-stage stochastic mixed-integer linear fraction programming (SMILFP) model. The objective is to minimize the expected levelized cost of energy (LCOE) under all the realization of scenarios, which is normally regarded as the cost at which energy must be generated to break-even over the life time of the project. The stochastic program is known for its computationally challenging property, because its problem size scales up exponentially as the number of scenarios increases. Therefore, a sample average approximation approach is applied to generate scenarios based on real EUR distribution data. Additionally, a novel algorithm integrating the parametric algorithm and the L-shaped method is

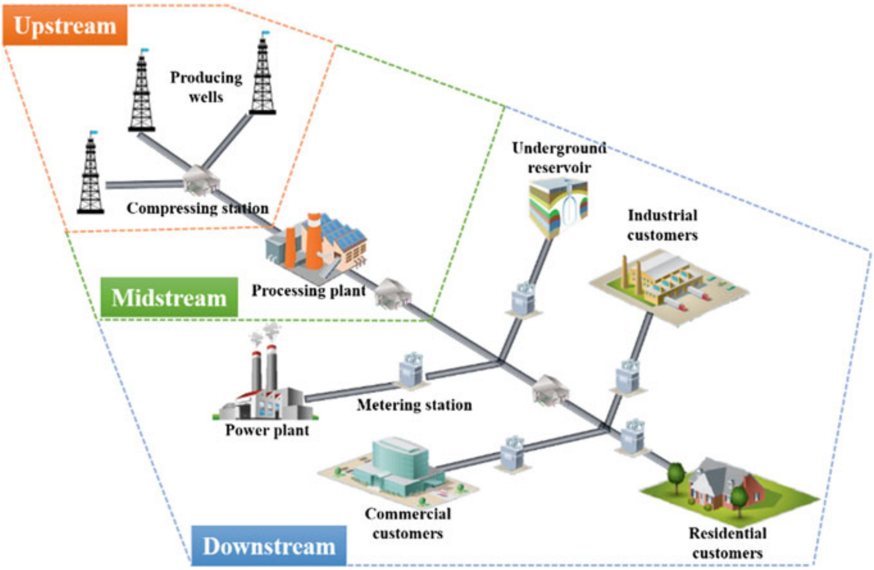

Fig. 2.2 Shale gas supply chain network from shale well to end-user (Gao and You 2015)

developed to solve the resulting large-scale SMILFP problem. The proposed modeling framework and solution method are demonstrated by a case study based on the Marcellus shale play. By solving the corresponding optimization problem, an LCOE of $0.0038/MJ is obtained. Moreover, by comparing the result with that of the perfect information model (all the EUR data are known beforehand), the LCOE is only 3 % less in the stochastic model. Meanwhile compared with the deterministic model (using nominal EUR data to determine design decisions), the LCOE obtained from the stochastic model is improved by 30 %. This result verifies the great influence of EUR uncertainty on the shale gas supply chain optimization, and the stochastic programming model is proven a superior choice for determining optimal shale gas supply chain design under EUR uncertainty.

Recently, Drouven and Grossmann (2016) propose multi-period planning, design and strategic models addressing the long-term quality-sensitive shale gas development problem. As important extensions of the previous work by Cafaro and Grossmann (2014), some new developments are presented. First, a novel superstructure for shale gas development problem is proposed, which captures the distinctive "tree"-structure of typical shale gas gathering system. Different delivery options including processing sales routes and direct delivery sales arcs are explicitly distinguished. In addition, discrete sizes of pipeline diameters and compressors are considered. Thus, the corresponding capacity constraints are captured by mixed-integer linear constraints, and the economies of scale is taken into account without involving concave cost functions. Moreover, this work extends the scope of shale gas development problem to include strategic decisions, such as the selection of delivery nodes, arrangement of delivery agreements, and procurement of delivery capacity. Most importantly, the spatial composition variations of shale gas are explicitly addressed in this work. The quality of shale gas is required to satisfy the delivery specifications at delivery nodes. Besides, depending on the price forecast, the upstream operator will target different shale gas qualities. The resulting problem is a large-scale, nonconvex, MINLP problem with an objective to maximize the NPV over the planning horizon. Based on the results, the shale gas development is proven to be quality sensitive. Additionally, the profitability of shale gas development projects can be improved by a few million U.S. dollars through the optimization of return-to-pad operations, equipment utilization, and strategic delivery agreements.

2.3 Sustainable Design and Operations of Shale Gas Supply Chain

Although the shale gas industry is well known for its great economic potential, another aspect that needs at least equal attention is its overall sustainability performance. There are two major topics focusing on the environmental impacts of shale gas development, namely the water management issue and the life cycle environmental impacts of shale gas. In this section, we provide a comprehensive description of the related problems and give a selected review of the recent optimization literature.

2.3.1 Water Management in Shale Gas System

Water use is associated with each step of drilling and shale gas production process. It is known that the hydraulic fracturing operation requires millions of gallons of freshwater (Jiang et al. 2014). In the Eagle Ford play of south Texas, for instance, large consumption of water resources in hydraulic fracturing would make the droughts even worse (Mauter et al. 2014). In other regions, such as Marcellus where water scarcity is not a severe problem, spatial and seasonal variability in stream flow rates still raises the risk that water withdrawals may negatively impact water resources (Mauter and Palmer 2014). Furthermore, as fracturing fluid is injected underground, a portion of water will flow back to the surface as highly contaminated water. The management of the flowback water and produced water is recognized as a greater challenge.

2.3.1.1 Overview of Water Management Options

The wastewater generated in shale gas development typically contains the following compositions: dissolved salts, minerals, residual fracturing fluid additives, heavy metals, bacteria, suspended solids, naturally occurring radioactive material, volatile organics, hydrocarbons, and ammonia (Karapataki 2012). In general, this water can be classified by the amount of total dissolved solids (TDS) per liter. Based on the operational definition, water produced during the well completion stage is defined as flowback water. On the other hand, water is referred to as produced water when the well is under production. Notably, 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 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 (Slutz et al. 2012; Gaudlip and Paugh 2008). The wastewater can be handled in multiple ways: direct injection into the Class II disposal wells, centralized wastewater treatment, and onsite treatment for reuse in hydraulic fracturing operations (Slutz et al. 2012; Veil 2010). These options are briefly introduced in the following sections.

Class II Disposal Wells

Disposal wells for injection of brine associated with oil and gas operations are classified as Class II disposal wells. We use disposal wells for abbreviation in the rest of this chapter. The wastewater from shale gas production can be directly sent to disposal wells and pumped into deep impermeable rock layers. This option is chosen when nearby disposal wells are available and permitted for underground injection. For states where disposal wells are abundant, the underground injection is a cost-effective option. If it is not the case, such as Marcellus in Pennsylvania where only several disposal wells are reported with limited capacity, wastewater will have to be transported to out-of-state locations, such as Ohio, for disposal, making this option much less attractive due to high transportation cost. Additionally, the underground injection option is criticized for the risks of causing water contamination and inducing seismicity (EPA 2011; Vidic et al. 2013). Therefore, the application of underground injection must be strictly subject to corresponding well capacity and regulations in case of unexpected environmental issues.

Centralized Wastewater Treatment Facility

The wastewater from shale gas production can also be transported to centralized wastewater treatment (CWT) facilities for treatment. The treated water is then discharged to surface water or recycled to shale sites for reuse. The resulting concentrated brine is sent to underground injection or taken down to zero liquid discharge condition and disposed as solid waste (API 2010; Puder and Veil 2006). CWT facilities involve a sequence of treatment processes. In general, the first step is fine particle filtration where the wastewater is screened to remove large objects, and then water is pumped into settling tanks to allow settling of heavy solids and removal of free oil. The second step is softening, where feedstock goes through agitation, aeration, pH adjustment, etc. to soften the water. The third step is ultrafiltration, where particulates and macromolecules are removed. This step is followed by reverse osmosis/nanofiltration/thermal distillation, where most salts and other effluent materials are removed. Finally, certain toxic elements such as boron are removed to meet the specifications of surface discharge or reuse (Veil 2010). The advantages of CWT treatment option are its lower treatment cost compared with onsite treatment option and the potential to reduce freshwater consumption by recycling. However, the economic viability of this option depends on the proximity of CWT facilities to shale sites as well.

Onsite Treatment for Reuse
The last option is onsite treatment for reuse, where some mobile water treatment units are installed at shale site to treat the wastewater. There are three levels of onsite treatment, each of which corresponds to different technologies and treatment results (Veil 2010; Acharya et al. 2011). The primary treatment is all about clarification, where suspended matter, free oil and grease (FOG), iron, and microbiological contaminants are removed. Technologies for primary treatment include coagulation, flocculation and disinfection, electro-coagulation microfiltration/ultrafiltration, adsorption, ozonation, etc. The secondary treatment involves softening, where harness ions are removed. The corresponding technologies include lime softening, ion exchange, activated carbon, and so on. The tertiary treatment focuses on desalination to reduce the TDS. Major technologies for tertiary treatment include membrane separation, electrically driven membrane separation, thermal distillation, and zero liquid discharge. Since the primary and secondary treatments only partially treat the wastewater, a certain amount of make-up water is required for blending to satisfy the reuse specification for TDS concentration. For tertiary treatment, blending with freshwater is considered as a way of pretreatment to reduce the TDS concentration, so that the feed water can be treated more effectively.

2.3.1.2 Optimization Models for Water Management

Most existing publications addressing water management problem focus on evaluating the environmental impacts of hydraulic fracturing and providing techno-economic analysis of specific water management options (Slutz et al. 2012; Vidic et al. 2013; Goldstein 2014; McHugh et al. 2014; Horner et al. 2011). However, considering the shale water supply chain as a complex system that involves numerous technology alternatives, it is important to develop an integrated approach to address all the challenges and opportunities of the water-energy system simultaneously.

Yang et al. (2014) first propose an optimization model for shale gas water management. Key aspects for water use in hydraulic fracturing, including source water acquisition, wastewater production, reuse and recycle, subsequent transportation, storage, and disposal are considered. A discrete-time two-stage stochastic MILP model is proposed to address the uncertainty of water availability. In this work, two specific problems are considered. The first problem mainly focuses on the water acquisition stage, and the goal is to find the optimal water acquisition strategy regarding different water sources. The uninterruptible sources are available throughout the year but require expensive truck transportation. The interruptible sources can be transported by pipeline with lower cost but are affected by seasonal availability. Storage option is also taken into account to coordinate water acquisition and demand. The objective is defined as minimizing the expected trucking and pumping cost of the water required to complete all the well sites. According to the optimization results of an example case, the total expected cost is reduced by $2.4 million compared against a heuristic schedule. The second problem addresses a more comprehensive model, where the handling of wastewater and revenue from gas production are taken into account. The goal is to determine the optimal fracturing schedule, as well as logistics for water acquisition, flowback reuse, and treatment. The objective is maximizing the expected profit from shale gas production after considering the operating cost for water management. Through this optimization, the expected profit is increased by 37 % from $156.41 million to $214.15 million, and the total cost is reduced from $25.02 million to $23.41 million compared to the heuristic schedule. Notably, this work is later extended by Yang et al. (2015) to optimize the long-term investment decisions using a deterministic MILP model. Multiple design decisions including capacity of water impoundments, pipeline options, treatment technologies and facility locations, as well as the fracturing schedule are addressed.

In order to explore more sustainable solutions for the shale water management. Gao and You (2015) develop a novel modeling framework for integrated design and operations of a water supply chain network for shale gas production. In this work, both the strategic design decisions (selection of freshwater sources, selection of transportation modes and capacities, installation of onsite treatment facilities, etc.), and operational decisions (water acquisition, water treatment, storage and transportation, etc.), are considered. Tradeoff between cost effectiveness and freshwater conservancy is captured with explicit consideration of multiple water management options and corresponding technologies. A novel fractional objective function is considered, which reflects the profit associated with unit net consumption of freshwater. The resulting problem is formulated as an MILFP and further solved by some tailored solution algorithms. To demonstrate the advantage of the proposed MILFP model, an MILP model targeting for maximizing the total profit is considered for comparison. By solving a large-scale case study based on Marcellus shale play, the results show that: (1) By consuming the same amount of freshwater resource, the MILFP model generates 14 % more profit and saves 12 % net water consumption than the MILP model. (2) Although the CWT is more cost effective in terms of water treatment, the onsite treatment option generates more balanced solution with better water efficiency, and the resulting reduction in water consumption can be significant. (3) The optimal water management strategy can be variant depending on the specific shale play and corresponding regulations (e.g. see Fig. 2.3 for the results obtained from the MILFP model).

Recently, Lira-Barragán et al. (2016) present a mathematical programming formulation for synthesizing water networks associated with shale gas hydraulic fracturing operations while accounting for uncertainties. The uncertainties

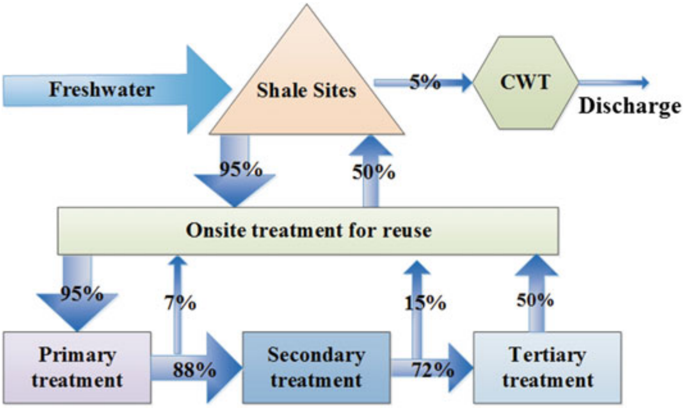

Fig. 2.3 Optimal water management strategy for MILFP model (Gao and You 2015)

correspond to the water requirements to fracture each well and the portion of this water that returns as flowback water. A two-stage stochastic programming model is developed and solved to minimize the total expected annual cost. The goal of the introduced approach is to provide guidance for decision makers in managing water resources and in acquiring properly sizes for water management systems. Meanwhile, Lira-Barragán et al. (2016) propose a similar model formulation to include the water consumption in the optimization. The economic objective function consists of the minimization of the total annualized cost, and the environmental goal aims at minimizing the total fresh water requirements.

2.3.2 Life Cycle Optimization of Shale Gas Supply Chains

The life cycle carbon footprint of shale gas is another popular topic that has been extensively addressed by using life cycle assessment approaches (Weber and Clavin 2012; Heath et al. 2014). Nevertheless, a research need of decision-support tools and methodologies dedicated to the sustainable design and operations of a shale gas supply chain system can be identified. To fill the knowledge gap in this research area, Gao and You (2015) develop a functional-unit-based life cycle optimization model for the optimal design and operations of shale gas supply chains. Such a shale gas supply chain covers the "well-to-wire" life cycle of shale gas, in which decisions regarding network design, drilling scheduling, water management, technology selection, facility location and sizing, natural gas storage, and transportation are fully captured. The levelized cost of electricity generated from shale gas is chosen as the economic indicator, and the environmental indicator is defined as GHG emissions per unit amount of electricity generation. A general superstructure of this shale gas supply chain is shown in Fig. 2.4.

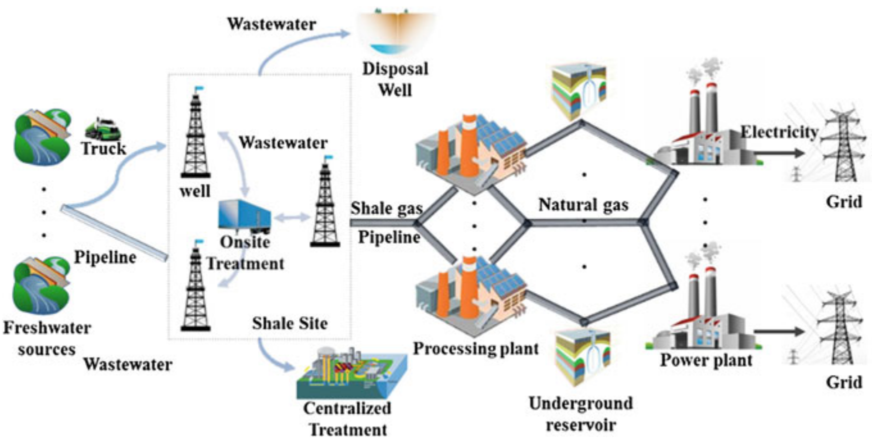

Fig. 2.4 Superstructure of the "well-to-wire" shale gas supply chain (Gao and You 2015)

The resulting problem is a multi-objective, multi-period MINLP problem, which is further solved by applying a tailored global optimization method integrating both the parametric algorithm and branch-and-refine approach. The proposed modeling framework and solution algorithm are demonstrated by a specific case study based on the Marcellus shale play in southwest PA. By solving this life cycle optimization problem, a Pareto-optimal curve consisting of 10 Pareto optimal solutions is obtained. The corresponding figure is presented in Fig. 2.5, which shows the trade-offs between the levelized cost of electricity and unit GHG emissions.

As can be seen in Fig. 2.5, point A has the lowest GHG emissions per unit electricity generation of 443 kg CO_2e/MWh, and it has the highest levelized cost of

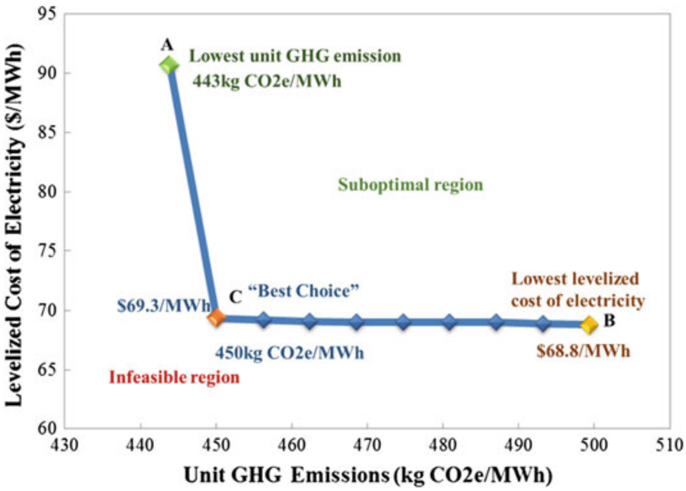

Fig. 2.5 Pareto-optimal curve of the shale gas supply chain (Gao and You 2015)

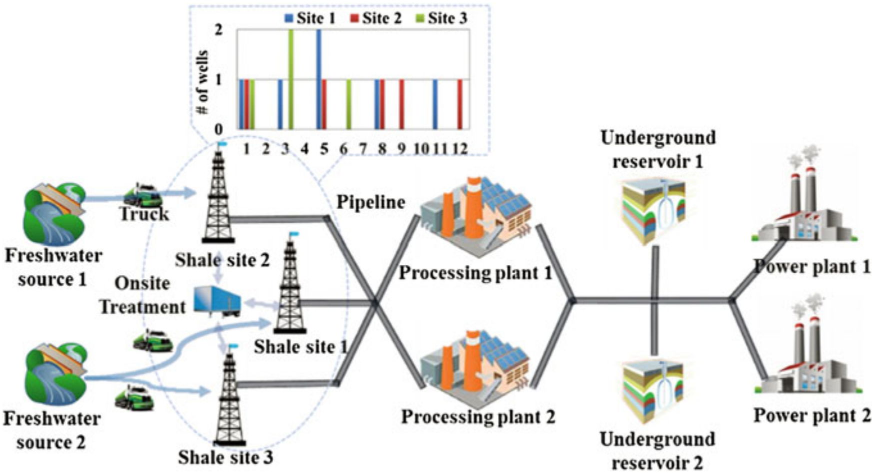

Fig. 2.6 Optimal shale gas supply chain strategies for "Best Choice" solution (Gao and You 2015)

electricity of \$69/MWh. Point B has the lowest levelized cost of electricity of \$69/MWh and the highest GHG emissions per unit electricity generated of 499 kg CO_2e/MWh. Point C is considered as the "best choice" solution, whose levelized cost of electricity is \$69/MWh and unit GHG emissions us 450 kg CO_2e/MWh. By reviewing the cost and emission breakdowns, we identify the power generation as the primary source of GHG emissions, and the shale gas production and processing contribute to the largest portion of total cost. The optimal shale gas supply chain strategies for the "Best Choice" (point C) are given in Fig. 2.6.

The optimal strategies can be summarized by the following points: (1) Trucks are more flexible and cost-effective option for freshwater transportation considering the life cycle performance. (2) More pipeline links can potentially improve the overall economic performance of shale gas supply chain in the long term. (3) A relatively "evenly-distributed" shale well drilling schedule is the key to maintain a stable shale gas production profile, and thus benefiting the overall supply chain performance. (4) Managing wastewater with reverse osmosis (RO) technology onsite is identified as the most sustainable wastewater treatment strategy. (5) Underground reservoirs are important "buffers" coordinating the drilling activities and market demand for a better economic performance.

2.4 Shale Gas Processing and Conversion

The previous sections mainly discuss the supply chain optimization problems in shale gas industry. In this section, we focus on the shale gas processing optimization from a process design perspective. Potential opportunities regarding co-production of various chemicals from shale gas feedstock are discussed.

2.4.1 Shale Gas Processing Plant

A general design for the conventional shale gas processing plant is presented in Fig. 2.7. As shown below, first the raw shale gas pipelined from wellheads goes through a gas sweetening section, where the acid impurities, such as H_2S and CO_2, are removed. Considering the mutable characteristic of shale gas composition, three alternative schemes are employed to efficiently neutralize the raw gas as follows: (1) when the gas is only slightly sour, fixed-bed type scavenger process would be a cost-effective approach to H_2S removal; (2) chemical absorption-based acid gas removal (AGR) process followed by a scavenger process, works well for raw gas with moderate to high content of CO_2 and small content of H_2S; and (3) for moderate amounts of H_2S, the sulfur must be captured by a sulfur recovery unit when its amount exceeds a limit specified by the environmental regulations (Parks et al. 2010). The shale gas input after the gas sweetening is considered as sweet gas, which will pass through a dehydration section to remove the water vapor typically using the regenerable adsorption in liquid triethylene glycol. Next, a NGL recovery section uses a turbo-expansion configuration combined with an external refrigerant designed to recover about 80 % of the ethane from the dry gas. As seen in this figure, the remaining gas (mainly methane) is finally compressed as pipeline gas or sent to an N_2 rejection section depending on the N_2 concentration; otherwise, high N_2 content (>4 mol%) would make the heating value of the pipeline gas lower than specified (Natural Gas Processing 2006). The nitrogen rejection process employs a cryogenic distillation unit integrated with a heat pump system. Besides, marketable NGL products including ethane, propane, butanes, and pentanes, etc. are sequentially extracted by passing through a fractionation train consisting of a deethanizer, a depropanizer, and a debutanizer. Likewise, some strict specifications on NGL products should be considered like Y-grade (Y-Grade Product Specifications 2012).

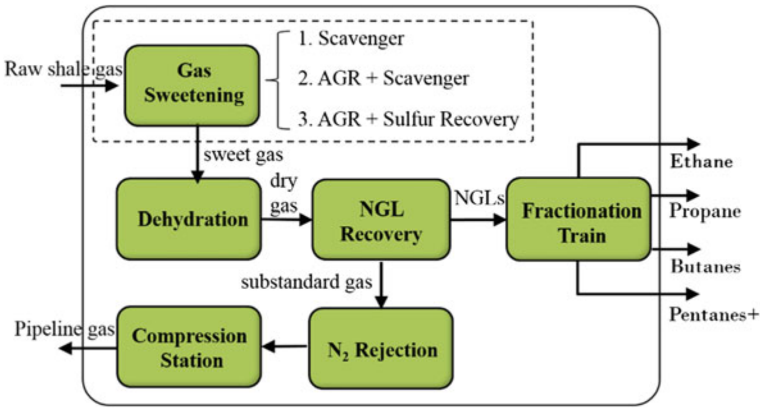

Fig. 2.7 Conventional shale gas processing plant

2.4.2 Shale Gas Conversion Scheme

Shale gas boom significantly increased interest in C_1, C_2, and C_3 chemistry to convert methane, ethane, and propane to value-added products, respectively, as shown in Fig. 2.8. In chemical industries, one-carbon-molecule compounds (like methanol, formaldehyde, formic acid, methylene chloride, etc.) tend to be derived from C_1 methane or carbon monoxide (itself derived from methane), two-carbon compounds (ethylene, acetaldehyde, ethanol, acetic acid, ketene, ethylene glycol, etc.) from C_2 ethane, three-carbon compounds (propylene, acetone, isopropyl alcohol, acrylic acid, etc.) from C_3 propane, and so on (Siirola 2014; Mitchell and Shantz 2015). In addition, chemicals with larger molecules could be formed through reactive functional groups including ether, esters, amides, etc. In particular, it is well-known that methane is always the dominant but less valuable ingredient in shale gas. The current industrial practice of steam reforming (SMR) produces syngas, which can be further used as an intermediate to produce other chemical commodities. Besides, methane and ethane are recognized as two major chemicals that potentially lead to integration opportunities with other chemical systems (He and You 2014; Ehlinger et al. 2014; Martín and Grossmann 2013). These opportunities include: (1) producing liquid fuels from methane, (2) producing methanol from methane, and (3) producing ethylene from ethane. This section focuses on relevant novel process designs and integrations and review of corresponding literature.

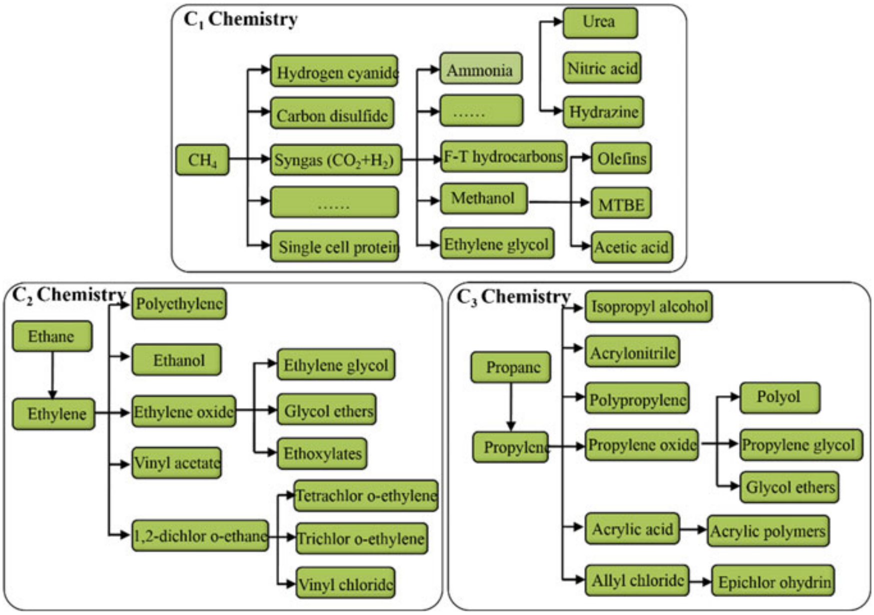

Fig. 2.8 Typical C_1, C_2, and C_3 production schemes (Siirola 2014)

To address the utilization of shale-derived natural gas, Martín and Grossmann (2013) present a superstructure optimization approach for the simultaneous production of liquid fuels and hydrogen from switchgrass and shale gas. This process is based on Fischer-Tropsch (FT) technology, in which shale gas is reformed with steam, while the switchgrass is gasified and reformed. After the raw gas is cleaned up and its composition is adjusted, the sour gases are removed. Finally, the liquid fuels, namely fuel gas, gasoline, and diesel, are produced using an FT reactor. By implementing a superstructure optimization approach, this integrated production system is able to achieve a production cost lower than \$1/gal if biomass price is below \$100/t and shale gas price is below \$11.5/MMBTU.

In addition to producing liquid fuels from natural gas. Ehlinger et al. (2014) present a shale gas processing design that aims to produce methanol with shale gas feedstock. The raw shale gas has to undergo a set of preprocessing steps, including acid gas removal, dehydration, and nitrogen removal. Then the "pipeline quality" gas can be sent to a methanol plant as feedstock. In order to produce methanol, the first step is to produce syngas, which can be achieved via partial oxidation, stream reforming, or autothermal reforming. In another work by Noureldin et al. (2014), an optimization-based model is proposed targeting on modeling and selection of reforming approaches for syngas generation from natural/shale gas. In this work, the partial oxidation is selected as the reforming technology. After going through the partial oxidation reactor, vapor-liquid equilibrium separator (VLE-SEP), water-gas shift reactor (WGS), another VLE-SEP, and a CO_2 separator, the syngas is obtained and ready for the methanol production. The methanol synthesis occurs as a combination of two reactions in the syngas mixture in the MeOH reactor under low temperatures (503–533 K) and high pressures (50–100 atm).

$$CO_{(g)} + H_2O_{(g)} \leftrightarrow H_{2(g)} + CO_{2(g)} \quad \Delta H^{298} = -41\,\text{kJ/mol} \tag{1}$$

$$CO_{2(g)} + 3H_{2(g)} \leftrightarrow CH_3OH_{(l)} + H_2O_{(g)} \quad \Delta H^{298} = -50\,\text{kJ/mol} \tag{2}$$

By conducting a techno-economic analysis based on the gas-to-methanol process, production of methanol from shale gas is proven to be profitable for a broad range of methanol selling price and shale gas costs. A desirable 31 % ROI can be achieved in the case study. Following this work, an extensive economic and environmental analysis for the production of methanol from shale gas is presented (Julián-Durán et al. 2014), in which four types of reforming technologies, namely partial oxidation, steam methane reforming, autothermal reforming, and combined reforming are considered. The partial oxidation and autothermal reforming are identified with better economic performances, while the combined reforming outperforms other alternatives with the best environmental performance.

Apart from methane, ethane is an important feedstock for ethylene production. Therefore, integration between shale gas processing and ethylene production is another popular research direction. He and You (2014) propose three novel process designs for integrating shale gas processing with ethylene production. These novel process designs include shale gas sequential processing (SSP), ethane cracking gas (a processable mixture including C_2H_4, H_2, C_2H_6, CH_4, etc.) recycling to NGL recovery (CRN), and cracking gas recycling to dehydration (CRD) designs. A unique feature of the proposed process designs is the co-processing strategy of shale gas and cracking gas. The SSP design has an identical processing structure as that of a conventional shale gas processing plant, but the ethane extracted from NGLs is pipelined to a local ethylene plant as feedstock. In the ethylene plant, ethane is converted into cracking gas using thermal steam cracking technology. The cracking gas then passes through the dehydration area, followed by a cracking gas separation area where ethylene and other products are produced and unconverted ethane is recycled. The CRN design adopts a modified NGL recovery section and fractionation train section. As a result, the cracking gas from ethylene plant can be co-processed by the modified area with dry gas after the dehydration area. Moreover, the cracking gas separation area can be eliminated from this design. The CRD design considers another recycling strategy, in which the produced cracking gas together with sweet gas are introduced to a centralized dehydration area for further purification and separation. Compared with the CRN design, the dehydration area in the ethylene plant is removed. Based on the proposed shale gas processing designs, the authors develop detailed thermo-economic models and energy analysis for the process designs. The economic analysis reveals that the estimated NPVs in the proposed SSP, CRN, and CRD designs are 1.7–2.4 times greater than that of conventional processing design. Furthermore, the NGL-richer shale gas generally produces 3.17–5.12 times estimated NPV than NGL-leaner shale gas.

Following this work, the authors extend the scope and further develop a novel process design for making chemicals from shale gas and bioethanol (He and You 2015). Such a process design consists of four major process areas: gas treatment, gas to chemicals, methane-to-ethylene, and bioethanol-to-ethylene. As always, the gas treatment aims to purify the raw shale gas, where acid gas and water vapor are either removed or recovered, and dry gas is ready to enter the next process area, namely the gas to chemicals area. In this area, heavy NGLs (butanes and natural gasoline) and low-boiling gases (methane, H_2, etc.) are successively taken from the dry gas using an NGL cutting unit. The C_2 and C_3 hydrocarbons in the remaining steam are then sent to an olefin separation unit followed by an olefin production unit. Meanwhile, the H_2-rich gas goes through a pressure swing adsorption (PSA) unit for hydrogen recovery. Next, methane from the NGL cutting unit is sent to the methane-to-ethylene area and then partially oxidized via the oxidative coupling of methane (OCM) reaction in an O_2-rich environment. The OCM product includes ethylene, ethane, hydrogen, carbon dioxide, carbon monoxide, and unconverted methane. Finally, in the bioethanol-to-ethylene area, bioethanol is used as a renewable feedstock for producing ethylene with tail gas from PSA as the dehydration fuel. Such a shale gas process design is further optimized by using a simulation-optimization method based on the NSGA-II algorithm. In the "good choice" optimal design, the minimum ethylene selling price can be reduced to \$877.2/ton, and the unit GWP of ethylene is 0.360 kg CO_2-eq/kg in the high carbon shale gas scenario. In the low carbon scenario, the results are \$655.1/ton and

0.030 kg CO_2-eq/kg, respectively. The results reveal that shale gas can be converted to more cost-effective and greener chemicals with proper process design, integration, and optimization.

Most recently, in order to decipher the true production costs and environmental impacts of shale gas-to-olefin (STO) projects, He and You (2016) develop a mega-scale shale gas supply chain olefin production network model with explicit consideration of process designs, integration methods, and alternative technologies. A techno-economic-environmental life cycle analysis is conducted for systematically evaluating the energy-water-carbon nexus. Four major shale regions of the U. S., including Appalachian, Gulf Coast, Mid-Continent, and Rocky Mountain regions are considered. A total of 594,922 shale wells are involved. In the proposed STO process, the petrochemical plant is co-located with shale plays and gas processing facilities. The raw shale gas is processed in multisite distributed processing facilities, and the recovered NGLs are moved to a centralized steam cracking plant, where the NGLs are fractionated and pyrolyzed. The results obtained from this work indicates that the STO located at the Mid-Continent region has relatively low environmental impacts. Besides, shale gas is still a low-carbon feedstock though its GHG emissions are 15 % higher than NG-ethane on average. Based on the sensitivity analysis, the well lifetime is identified as the critical factor in evaluating the overall environmental footprints.

In addition to the aforementioned processes and integrations, there are multiple alternatives that remain to be further expanded. For instance, Wang et al. (2013) propose a highly efficient cold energy integrating scheme by integrating NGL recovery from shale gas and LNG regasification at receiving terminals. The goal of this study is to recycle the cold energy from LNG regasification process to assist the NGL recovery process for economic improvement and energy saving. A general methodology framework is proposed and further decomposed into four steps: the first step is to develop the process superstructure and prepare corresponding data; then, a simulation-assisted MILP model is developed and solved for the optimal process synthesis; next, heat exchange network design and analysis are performed based on the pinch technology to accomplish the maximum energy saving target; finally, rigorous plant-wide simulations are conducted to validate the feasibility and capability of the entire process design coupling of separation and heat integration. By comparing the optimal integrated design proposed in this work with independent LNG regasification and NGL recovery processes, the authors observe a 61.8 % reduction in hot utility and 100 % reduction of cold utility.

2.5 Future Directions

Although the shale gas industry has been developed for decades, there are many research challenges on applying mathematical programming tools for shale gas process and supply chain optimization problems. These challenges include, but are not limited to: optimization of shale gas system under uncertainty, modeling and optimization of shale gas supply chain from a non-cooperative perspective, and multi-scale optimization integrating shale gas supply chain and processing system.

First, uncertainty is ubiquitous in shale gas supply chains. Multiple uncertainties have been identified with significant influence on the overall performance of shale gas system, such as freshwater availability, EUR of shale wells, composition of shale gas, and price of natural gas. Despite the great importance of hedging against uncertainty, most of the existing literature either fail to capture such a key issue or only consider some types of uncertainties that are easy to address. With the recent development of optimization techniques, such as multi-stage robust optimization and data-driven stochastic programming, we expect more modeling frameworks and applications to be proposed in the optimization of shale gas system under various uncertainties.

Besides, a shale gas supply chain could consist of multiple stakeholders, such as the upstream shale producers, midstream processors, and downstream distributors and customers. In general, each of them pursues its own objective and makes decisions independently. Nevertheless, almost all of the existing studies rely on the cooperative shale gas supply chain model, in which a single decision maker is assumed to have full control of the entire system. Consequently, the optimal strategy obtained from a centralized model can be practically infeasible. In order to better capture the performance of a shale gas supply chain, it is necessary to properly address the non-cooperative relationship between multiple stakeholders in shale gas supply chain optimization problems.

Last, shale gas process design and supply chain optimization are both important problems with different spatial scales. Research addressing each of the systems has unveiled great economic and environmental benefits. However, there is no modeling framework addressing shale gas process design and supply chain management simultaneously for better economic and environmental performances. By developing a holistic systematic approach to integrate these two systems, it will lead to better overall performance and more potential design alternatives that can facilitate the development of shale gas industry.

2.6 Conclusion

This chapter provides a comprehensive introduction on the shale gas supply chain and processing system. Major research areas including the optimal design and operations of shale gas supply chain, water management and emission mitigation in shale gas development, and novel shale gas processing designs and integrations are identified. Corresponding literature is reviewed and discussed in details. Furthermore, potential research opportunities are summarized, including optimization under various uncertainties, modeling and optimization of non-cooperative supply chain, and simultaneous optimization of shale gas supply chain and process systems.

References

Acharya, H. R., Henderson, C., Matis, H., Kommepalli, H., & Wang, H. (2011). *Cost effective recovery of low TDS frac flowback water for re-use*. Niskayuna, NY 12309-1027: Department of Energy.

Allen, D. T. (2014a). Methane emissions from natural gas production and use: Reconciling bottom-up and top-down measurements. *Current Opinion in Chemical Engineering, 5*, 78–83. doi:10.1016/j.coche.2014.05.004.

Allen, D. T. (2014b). Atmospheric emissions and air quality impacts from natural gas production and use. *Annual Review of Chemical and Biomolecular Engineering, 5*(1), 55–75. doi:10.1146/annurev-chembioeng-060713-035938.

Alvarez, R. A., Pacala, S. W., Winebrake, J. J., Chameides, W. L., & Hamburg, S. P. (2012). Greater focus needed on methane leakage from natural gas infrastructure. *Proceedings of the National Academy of Sciences, 109*(17), 6435–6440. doi:10.1073/pnas.1202407109.

API. (2010). *Water management associated with hydraulic fracturing*. Institute AP.

Brandt, A. R., Heath, G. A., Kort, E. A., O'Sullivan, F., Pétron, G., Jordaan, S. M., et al. (2014). Methane leaks from North American natural gas systems. *Science, 343*(6172), 733–735. doi:10.1126/science.1247045.

Burnham, A., Han, J., Clark, C. E., Wang, M., Dunn, J. B., & Palou-Rivera, I. (2011). Life-cycle greenhouse gas emissions of shale gas, natural gas, coal, and petroleum. *Environmental Science and Technology, 46*(2), 619–627. doi:10.1021/es201942m.

Cafaro, D. C., & Grossmann, I. E. (2014). Strategic planning, design, and development of the shale gas supply chain network. *AIChE Journal, 60*(6), 21. doi:10.1002/aic.14405.

Chaudhri, M. M. (2012). Numerical modeling of multifracture horizontal well for uncertainty analysis and history matching: Case studies from Oklahoma and Texas shale gas wells.

Chima, C. M. (2011). Supply-chain management issues in the oil and gas industry. *Journal of Business & Economics Research (JBER), 5*(6).

Dale, A. T., Khanna, V., Vidic, R. D., & Bilec, M. M. (2013). Process based life-cycle assessment of natural gas from the Marcellus Shale. *Environmental Science and Technology, 47*(10), 5459–5466. doi:10.1021/es304414q.

DOE/NETL. (2011). Life cycle greenhouse gas inventory of natural gas extraction, delivery and electricity production.

Drouven, M. G., & Grossmann, I. E. (2016). Multi-period planning, design and strategic models for long-term, quality-sensitive shale gas development. *AIChE Journal*. doi:10.1002/aic.15174.

Duran, M., & Grossmann, I. (1986). A mixed-integer nonlinear programming algorithm for process systems synthesis. *AIChE Journal, 32*(4), 592–606.

Ehlinger, V. M., Gabriel, K. J., Noureldin, M. M. B., & El-Halwagi, M. M. (2014). Process design and integration of shale gas to methanol. *ACS Sustainable Chemistry & Engineering, 2*(1), 30–37. doi:10.1021/sc400185b.

EIA. (2011). *Review of emerging resources: U.S. shale gas and shale oil plays*. Washington, DC 20585: U.S. Energy Information Administration.

EIA. (2015). Annual Energy Outlook 2015 with projections to 2040. U.S. Energy Information Administration, Washington, DC 20585.

EIA Natural Gas Consumption by End Use. Retrieved June 16, 2015, from http://www.eia.gov/dnav/ng/ng_cons_sum_dcu_spa_a.htm.

EIA Underground Natural Gas Storage. Retrieved September 29, 2014, from http://www.eia.gov/pub/oil_gas/natural_gas/analysis_publications/ngpipeline/undrgrnd_storage.html.

EPA. (2011). *Plan to study the potential impacts of hydraulic fracturing on drinking water resources*. EPA, Washington, D.C.: Office of Research and Development U.S.

Gao, J., & You, F. (2015a). Deciphering and handling uncertainty in shale gas supply chain design and optimization: Novel modeling framework and computationally efficient solution algorithm. *AIChE Journal, 61*(11), 3739–3755. doi:10.1002/aic.15032.

Gao, J., & You, F. (2015b). Optimal design and operations of supply chain networks for water management in shale gas production: MILFP model and algorithms for the water-energy nexus. *AIChE Journal, 61*(4), 1184–1208. doi:10.1002/aic.14705.

Gao, J., & You, F. (2015c). Shale gas supply chain design and operations toward better economic and life cycle environmental performance: MINLP model and global optimization algorithm. *ACS Sustainable Chemistry & Engineering, 3*(7), 1282–1291. doi:10.1021/acssuschemeng.5b00122.

Gaudlip, A.W., & Paugh, L. O. (2008). Marcellus Shale water management challenges in Pennsylvania. *Paper presented at the shale gas Production Conference*. Fort Worth, Texas, 16–18 November.

Goldstein, B. D. (2014). The importance of public health agency independence: Marcellus shale gas drilling in Pennsylvania. *American Journal of Public Health, 104*(2), e13–e15. doi:10.2105/ajph.2013.301755.

Gracceva, F., & Zeniewski, P. (2013). Exploring the uncertainty around potential shale gas development—A global energy system analysis based on TIAM (TIMES Integrated Assessment Model). *Energy, 57*, 443–457. doi:10.1016/j.energy.2013.06.006.

Gregory, K. B., Vidic, R. D., & Dzombak, D. A. (2011). Water management challenges associated with the production of shale gas by hydraulic fracturing. *Elements, 7*(3), 181–186. doi:10.2113/gselements.7.3.181.

Gupta, V., & Grossmann, I. E. (2012). An efficient multiperiod MINLP model for optimal planning of offshore oil and gas field infrastructure. *Industrial and Engineering Chemistry Research, 51*(19), 6823–6840. doi:10.1021/ie202959w.

Harding, N. R. (2008). Application of stochastic prospect analysis for shale gas reservoirs.

Harto, C. (2013). *Management of water from CCS: Life cycle water consumption for carbon capture and storage* (trans: Energy USDo). Argonne National Laboratory.

He, C., & You, F. (2014). Shale gas processing integrated with ethylene production: Novel process designs, exergy analysis, and techno-economic analysis. *Industrial and Engineering Chemistry Research, 53*(28), 11442–11459. doi:10.1021/ie5012245.

He, C., & You, F. (2015). Toward more cost-effective and greener chemicals production from shale gas by integrating with bioethanol dehydration: Novel process design and simulation-based optimization. *AIChE Journal, 61*(4), 1209–1232. doi:10.1002/aic.14713.

He, C., & You, F. (2016). Deciphering the true life cycle environmental impacts and costs of the mega-scale shale gas-to-olefins projects in the United States. *Energy & Environmental Science, 9*, 820–840. doi:10.1039/C5EE02365C.

Heath, G. A., O'Donoughue, P., Arent, D. J., & Bazilian, M. (2014). Harmonization of initial estimates of shale gas life cycle greenhouse gas emissions for electric power generation. *Proceedings of the National Academy of Sciences, 111*(31), E3167–E3176.

Horner, P., Halldorson, B., & Slutz, J. A. (2011). Shale gas water treatment value chain—A review of technologies including case studies. In *SPE Annual Technical Conference and Exhibition*. Society of Petroleum Engineers.

Howarth, R. W. (2014). A bridge to nowhere: Methane emissions and the greenhouse gas footprint of natural gas. *Energy Science & Engineering, 2*(2), 47–60. doi:10.1002/ese3.35.

Hughes, J. D. (2013). A reality check on the shale revolution. *Nature, 494*(7437), 307–308.

Hughes, J. D. (2014). *Drilling deeper: A reality check on U.S. Government Forecasts for A Lasting Tight Oil & Shale Gas Boom*. California, Santa Rosa 95404: Post Carbon Institute.

Iyer, R. R., Grossmann, I. E., Vasantharajan, S., & Cullick, A. S. (1998). Optimal planning and scheduling of offshore oil field infrastructure investment and operations. *Industrial and Engineering Chemistry Research, 37*(4), 1380–1397. doi:10.1021/ie970532x.

Jayakumar, R., & Rai, R. R. (2012). Impact of uncertainty in estimation of shale gas reservoir and completion properties on EUR forecast and optimal development planning: A Marcellus case study.

Jiang, M., Hendrickson, C. T., & VanBriesen, J. M. (2014). Life cycle water consumption and wastewater generation impacts of a Marcellus shale gas well. *Environmental Science and Technology, 48*(3), 1911–1920. doi:10.1021/es4047654.

Julián-Durán, L. M., Ortiz-Espinoza, A. P., El-Halwagi, M. M., & Jiménez-Gutiérrez, A. (2014). Techno-economic assessment and environmental impact of shale gas alternatives to methanol. *ACS Sustainable Chemistry & Engineering, 2*(10), 2338–2344. doi:10.1021/sc500330g.

Karapataki, C. (2012). *Techno-economic analysis of water management options for unconventional natural gas developments in the Marcellus Shale*. Master thesis. Cambridge, MA 02139-4307: Massachusetts Institute of Technology.

Knudsen, B. R., & Foss, B. (2013). Shut-in based production optimization of shale-gas systems. *Computers & Chemical Engineering, 58*, 54–67. doi:10.1016/j.compchemeng.2013.05.022.

Knudsen, B. R., Grossmann, I. E., Foss, B., & Conn, A. R. (2014a). Lagrangian relaxation based decomposition for well scheduling in shale-gas systems. *Computers & Chemical Engineering, 63*, 234–249. doi:10.1016/j.compchemeng.2014.02.005.

Knudsen, B. R., Whitson, C. H., & Foss, B. (2014b). Shale-gas scheduling for natural-gas supply in electric power production. *Energy, 78*, 165–182. doi:10.1016/j.energy.2014.09.076.

Laurenzi, I. J., & Jersey, G. R. (2013). Life cycle greenhouse gas emissions and freshwater consumption of Marcellus Shale gas. *Environmental Science and Technology, 47*(9), 4896–4903. doi:10.1021/es305162w.

Lira-Barragán, L. F., Ponce-Ortega, J. M., Guillén-Gosálbez, G., & El-Halwagi, M. M. (2016a). Optimal water management under uncertainty for shale gas production. *Industrial and Engineering Chemistry Research, 55*(5), 1322–1335. doi:10.1021/acs.iecr.5b02748.

Lira-Barragán, L. F., Ponce-Ortega, J. M., Serna-González, M., & El-Halwagi, M. M. (2016). Optimal reuse of flowback wastewater in hydraulic fracturing including seasonal and environmental constraints. *AIChE Journal* n/a–n/a. doi:10.1002/aic.15167.

Martín, M., & Grossmann, I. E. (2013). Optimal use of hybrid feedstock, switchgrass and shale gas for the simultaneous production of hydrogen and liquid fuels. *Energy, 55*, 378–391. doi:10.1016/j.energy.2013.04.005.

Mauter, M., & Palmer, V. (2014). Expert elicitation of trends in Marcellus oil and gas wastewater management. *Journal of Environmental Engineering, 140*(5), B4014004. doi:10.1061/(ASCE)EE.1943-7870.0000811.

Mauter, M. S., Palmer, V. R., Tang, Y., & Behrer, A. P. (2013). 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.

Mauter, M. S., Alvarez, P. J. J., Burton, A., Cafaro, D. C., Chen, W., Gregory, K. B., et al. (2014). Regional variation in water-related impacts of shale gas development and implications for emerging international plays. *Environmental Science and Technology, 48*(15), 8298–8306. doi:10.1021/es405432k.

McHugh, T., Molofsky, L., Daus, A., & Connor, J. (2014). Comment on "an evaluation of water quality in private drinking water wells near natural gas extraction sites in the Barnett Shale formation". *Environmental Science and Technology, 48*(6), 3595–3596. doi:10.1021/es405772d.

Mitchell, S. F., & Shantz, D. F. (2015). Future feedstocks for the chemical industry—Where will the carbon come from? *AIChE Journal, 61*(8), 2374–2384. doi:10.1002/aic.14910.

Natural gas processing: The crucial link between natural gas production and its transportation to market (2006). Washington, DC: Energy Information Administration.

Nicot, J.-P., & Scanlon, B. R. (2012). Water use for shale-gas production in Texas, U.S. *Environmental Science and Technology, 46*(6), 3580–3586. doi:10.1021/es204602t.

Nicot, J. P., Scanlon, B. R., Reedy, R. C., & Costley, R. A. (2014). Source and fate of hydraulic fracturing water in the Barnett Shale: A historical perspective. *Environmental Science and Technology, 48*(4), 2464–2471. doi:10.1021/es404050r.

Noureldin, M. M. B., Elbashir, N. O., & El-Halwagi, M. M. (2014). Optimization and selection of reforming approaches for syngas generation from natural/Shale gas. *Industrial and Engineering Chemistry Research, 53*(5), 1841–1855. doi:10.1021/ie402382w.

Paper, W. (2008). *US shale gas—An unconventional resource, unconventional challenge*. Halliburton.

Parks, L. E., Perry, D., & Fedich, R. (2010). FLEXSORB ®SE A proven reliable acid gas enrichment solvent A2—Benyahia, Farid. In F. T. Eljack (Ed.), *Proceedings of the 2nd Annual Gas Processing Symposium* (Vol. 2, pp. 229–235). Amsterdam: Elsevier. doi:10.1016/S1876-0147(10)02025-2.

Puder, M. G., & Veil, J. A. (2006). *Offsite commercial disposal of oil and gas exploration and production waste: Availability, options, and costs* (trans: Division ES). Argonne National Laboratory for the U.S. Department of Energy, Office of Fossil Energy, National Energy Technology Laboratory.

Rahm, B. G., & Riha, S. J. (2012). Toward strategic management of shale gas development: Regional, collective impacts on water resources. *Environmental Science & Policy, 17*, 12–23. doi:10.1016/j.envsci.2011.12.004.

Seydor, S. M., Clements, E., Pantelemonitis, S., & Deshpande, V. (2012). *Understanding the Marcellus Shale supply chain*. Pittsburgh, PA 15260: University of Pittsburgh, Katz Graduate School of Business.

Siirola, J. J. (2014). The impact of shale gas in the chemical industry. *AIChE Journal, 60*(3), 810–819. doi:10.1002/aic.14368.

Slutz, J. A., Anderson, J. A., Broderick, R., & Horner, P. H. (2012). Key Shale gas water management strategies: An economic assessment. In *International Conference on Health Safety and Environment in Oil and Gas Exploration and Production*. Perth, Austrailia: Society of Petroleum Engineers.

Small, M. J., Stern, P. C., Bomberg, E., Christopherson, S. M., Goldstein, B. D., Israel, A. L., et al. (2014). Risks and risk governance in unconventional shale gas development. *Environmental Science and Technology, 48*(15), 8289–8297. doi:10.1021/es502111u.

Soeder, D. J., & Kappel, W. M. (2009). *Water resources and natural gas production from the Marcellus Shale*. Virginia: US Department of the Interior, US Geological Survey Reston.

Stephenson, T., Valle, J. E., & Riera-Palou, X. (2011). Modeling the relative GHG emissions of conventional and shale gas production. *Environmental Science and Technology, 45*(24), 10757–10764. doi:10.1021/es2024115.

Swindell, G. S. (2014). Marcellus Shale in Pennsylvania: A 2,600 well study of estimated ultimate recovery. *Paper presented at the SPE Annual Meeting*. Dallas, TX.

van den Heever, S. A., & Grossmann, I. E. (2000). An iterative aggregation/disaggregation approach for the solution of a mixed-integer nonlinear oilfield infrastructure planning model. *Industrial and Engineering Chemistry Research, 39*(6), 1955–1971. doi:10.1021/ie9906619.

Veil, J. A. (2010). *Final report water management technologies used by Marcellus shale gas producers*. Argonne, IL: Oil & Natural Gas Technology, U.S. Department of Energy.

Vengosh, A., Warner, N., Jackson, R., & Darrah, T. (2013). 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 (Vol. 14, No. 7, pp. 863–866). doi:10.1016/j.proeps.2013.03.213.

Vidic, R. D., Brantley, S. L., Vandenbossche, J. M., Yoxtheimer, D., & Abad, J. D. (2013). Impact of shale gas development on regional water quality. *Science, 340*(6134), 1235009. doi:10.1126/science.1235009.

Wang, M., Zhang, J., & Xu, Q. (2013). A novel conceptual design by integrating NGL recovery and LNG regasification processes for maximum energy savings. *AIChE Journal, 59*(12), 4673–4685. doi:10.1002/aic.14231.

Weber, C. L., & Clavin, C. (2012). Life cycle carbon footprint of Shale gas: Review of evidence and implications. *Environmental Science and Technology, 46*(11), 5688–5695. doi:10.1021/es300375n.

Yang, L., Manno, J., & Grossmann, I. E. (2014). Optimization models for shale gas water management. *AIChE Journal*. doi:10.1002/aic.14526.

Yang, L., Grossmann, I. E., & Manno, J. (2014b). Optimization models for shale gas water management. *AIChE Journal, 60*(10), 3490–3501. doi:10.1002/aic.14526.

Yang, L., Grossmann, I. E., Mauter, M. S., & Dilmore, R. M. (2015). Investment optimization model for freshwater acquisition and wastewater handling in shale gas production. *AIChE Journal, 61*(6), 1770–1782. doi:10.1002/aic.14804.

Y-Grade Product Specifications. (2012). ETC NGL Transport LLC. http://www.energytransfer.com/documents/UniformY-GradeSpecs-ETCV111612.pdf.

Zavala-Araiza, D., Allen, D. T., Harrison, M., George, F. C., & Jersey, G. R. (2015). Allocating methane emissions to natural gas and oil production from shale formations. *ACS Sustainable Chemistry and Engineering, 3*(3), 492–498. doi:10.1021/sc500730x.

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