Mathematical Optimization Models for Shale Oil & Gas Development: A Review and Perspective

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Abstract

In this paper, we provide a comprehensive review of optimization models for shale oil and gas development, and we offer a perspective on outstanding research opportunities. We distinguish contributions in five major topic areas, namely: (1) development planning, (2) water management, (3) production optimization, (4) supplies, gathering & processing, and (5) life cycle analysis & sustainability. We highlight how various types of mathematical programming models (i.e., linear programs, nonlinear programs, mixed-integer linear programs, mixed-integer nonlinear programs) have been proposed by the process systems engineering community to address the respective decision-making problems, and we highlight instances of successful deployment in industry. Finally, based on a critical assessment of the existing body of work, we identify opportunities for future research across the major topic areas.

1. Introduction

The development of optimization models to support decision-making processes in the unconventional oil and gas industry has primarily been driven by the "shale revolution". Just as conventional natural gas reserves declined in many countries around the globe, shale gas emerged as a key resource in the energy transition to a cleaner matrix. According to the International Energy Agency (IEA, 2019) coal-to-gas switching, mainly in the U.S., has reduced CO_2 emissions by 500 million tons, which is comparable to the impact of adding 200 million electric vehicles running on zero-carbon electricity over the same period. At the same time, it is important to note that this switching, on its own, does not provide a long-term resolution to climate change, and it is worth highlighting that coal has consistently remained in second place in the global energy mix, growing from 16% in 1971 to 23% in 2019 (IEA, 2019).

The need for computational tools to aid the sustainable development of shale oil and gas resources remains high. In the developing world, for instance, strategic investments in new gas infrastructure could make essential energy supplies more affordable, particularly those that cannot be cost-effectively replaced by low-carbon alternatives, such as peak winter heating. An expansion of gas grids could eventually also enable the transportation of decarbonized gases (e.g., renewable methane or hydrogen) while simultaneously offering benefits in terms of energy security (IEA, 2019). Such infrastructure investments may ultimately also accelerate the ability to deploy carbon capture, utilization and storage technology, all of which will require proven decision-support tools to be optimally planned and operated.

But even in “established” shale development areas, there is a growing need for optimization-based decision-support tools. The respective industry is facing a dramatic increase in complexity: ever-more production units, processing facilities, gathering pipelines, treatment plants and development resources need to be managed simultaneously – all while continuously striving to improve environmental stewardship and the impact on local communities. Making “good” decisions about development activities has never been more difficult, and that reality is accelerating the adoption of mathematical optimization tools in practice.

Over the years, the academic community and industry practitioners have consistently reported that the mathematical optimization of shale oil and gas development activities can result in significant economic and environmental improvements. Drouven & Grossmann (2016) published the findings of a comprehensive, multi-year development planning optimization case study conducted with a large natural gas producer in the Appalachian Basin and concluded that an optimization-based approach to scheduling drilling, fracturing and production operations could have resulted in a $100MM increase in NPV. Two years later, a major shale gas producer, EQT Corporation, showcased how a produced water scheduling tool leveraging mathematical programming was expected to save the company $25-35MM per year while also reducing the number of water hauling truck trips substantially (EQT Co., 2019).

The goal of this review paper is first to provide a general introduction to shale oil and gas development, and the impact it has had on the energy landscape in the United States, on the production of petrochemicals, as well as on the reduction of CO_2 emissions. Next, the paper presents a comprehensive overview of optimization-based techniques for addressing major subproblems, namely, development planning, production optimization, supplies, gathering and processing optimization, water management, and life cycle analysis (LCA) and sustainability. A major objective is to also identify trends of linear vs. nonlinear models, general purpose vs. specialized solution strategies, and the extent to which they account for uncertainty. The paper concludes with a critical assessment of these techniques and the identification of opportunities for further research.

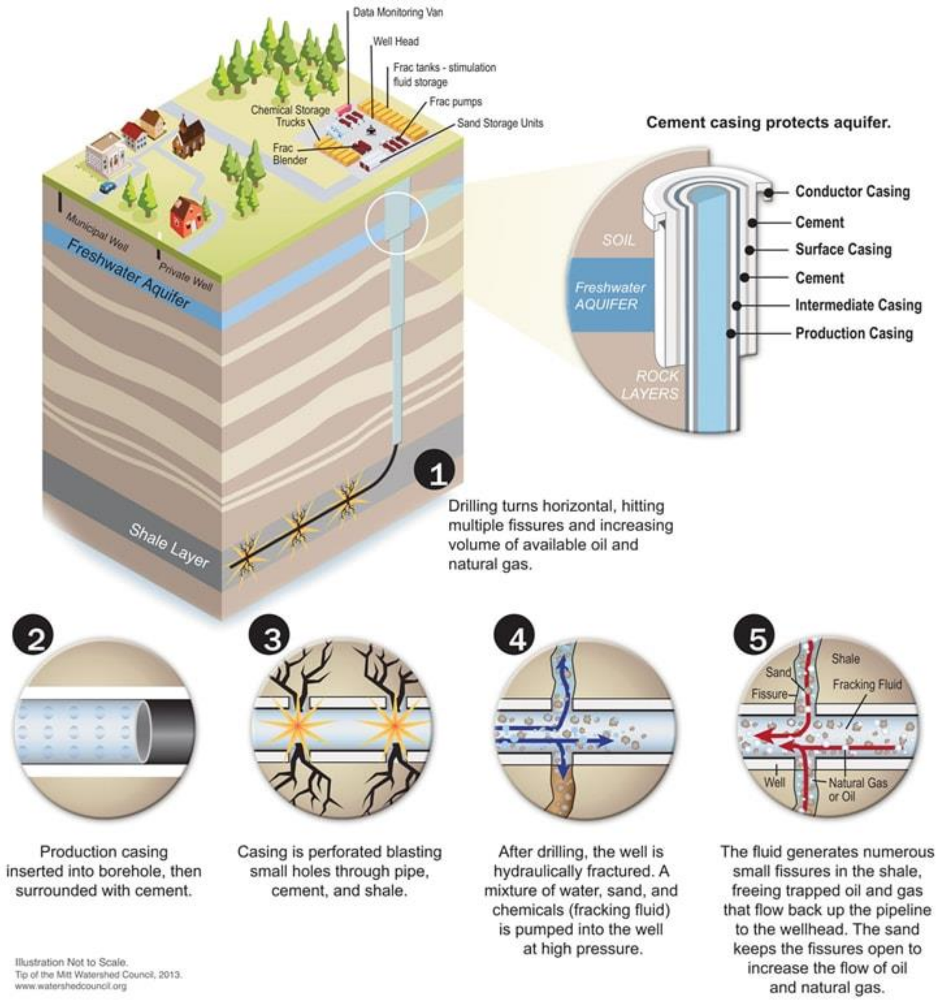


Figure 1. They hydraulic fracturing process explained
(Image source: https://www.watershedcouncil.org/hydraulic-fracturing.html)

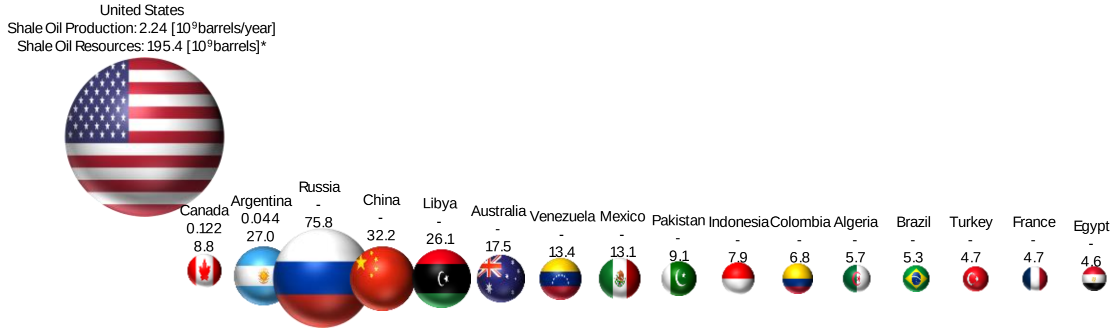
2. Background on Shale Oil and Gas Production and its Impact

Figure 1 shows the basic steps involved in developing a shale oil or gas well. The development process usually begins with the construction of a well site or "pad". This pad will house the temporary equipment necessary for drilling, hydraulic fracturing and ultimately producing hydrocarbons from one or many wells. Up to 60 wells may eventually originate from the surface of one single well pad. Well development itself begins by drilling the vertical section of the well which requires a special drilling rig, known as the "top-set" rig. Shortly before the wellbore reaches the depth of the target formation, the top-set rig is disassembled, and a second "horizontal" drilling rig is moved onsite. This rig can drill the horizontal segment of the shale well, which may stretch out several miles laterally underground. Well and production casing (i.e., layers of steel and cement) are placed during and after the drilling process to ensure the integrity of the well bore and prevent an uncontrollable collapse of the well. Eventually, that very casing is perforated using targeted explosions as part of wireline operations. These explosions create fractures that establish hydrocarbon flow pathways from the shale reservoir to the well itself. Finally, large volumes of water, proppant (i.e., specialized sand) and chemical additives are pumped into the well at very high pressures (up to 12,000 psi). This hydraulic fracturing step extends fissures into the shale rock (i.e., exposure to the hydrocarbon reservoir), which ultimately enables the flow of tight oil or natural gas into the well bore and up to the surface.

Figure 2. A representative shale well site showing a drilling rig and an adjacent water storage (Image source: https://www.kontextwochenzeitung.de/ueberm-kesselrand/78/gorleben-am-bodensee-981.html)

As production commences, a combination of oil, natural gas, proppant, and water is simultaneously brought to the surface. The ratio of these constituents varies over time and space (i.e., from one basin to the next). However, shale oil and gas wells are generally known for initially high production rates, that are followed by characteristically sharp (i.e., near-hyperbolic) declines in hydrocarbon flow. These declines lead to many "downstream" challenges including: (1) difficulties in maximizing equipment utilization (e.g., pipelines, compressor stations), (2) quick drop-offs in revenues related to hydrocarbon sales, and (3) a need for continuously opening up new wells to maintain production levels and honor commercial take-away commitments. In addition, shale wells produce considerable amounts of high-salinity water (so-called "produced water") once they are brought online. Total dissolved solids (TDS) concentrations in produced water range from 30,000 to 300,000 mg/L. This produced water must be transported off the well-site which creates considerable logistical and cost challenges in maintaining the production from shale wells. It is expected that shale wells will produce hydrocarbons and water for decades, even though production rates eventually taper off to minimal quantities of either.

2020 Shale Oil Production - where available- and 2013 Technically Recoverable Resources (10^9 barrels)



2020 Shale Gas Production - where available- and 2013 Technically Recoverable Resources (10^{12} scf)

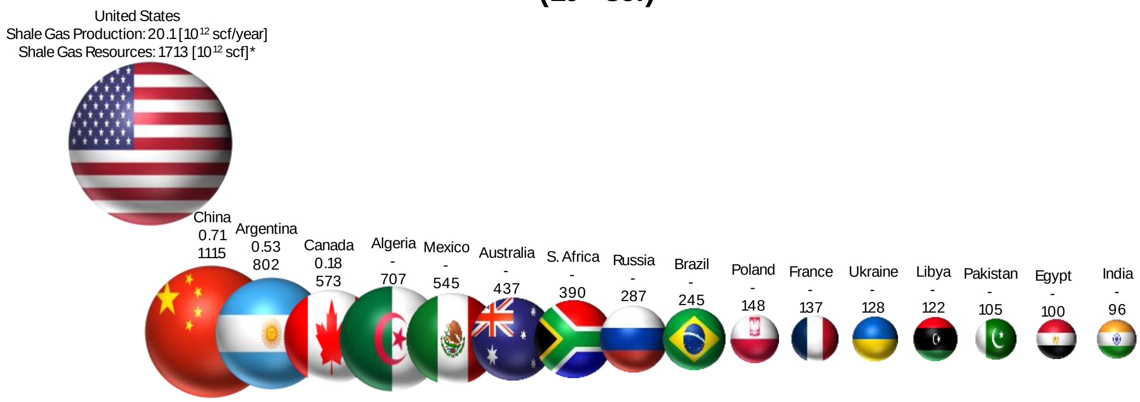


*Figure 3. Worldwide shale oil and shale gas production by 2020 (where data have been made available). Circles represent technically recoverable resources estimated by the U.S. EIA as of June 2013 (*except for the United States, for which estimations have been updated to 2020).*

The “shale revolution” has made accessible remarkable quantities of oil and natural gas across the world, but especially in the United States. In 2014, the U.S. Energy Information Administration assessed that “shale oil and shale gas resources were globally abundant” (EIA, 2014). The list of countries with access to considerable quantities of technically recoverable shale oil resources includes Russia, the United States, China, Argentina, Libya, Australia, Venezuela, Mexico, Pakistan, and Canada. Shale gas resources, on the other hand, are present in

China, Argentina, Algeria, the United States, Canada, Mexico, Australia, South Africa, Russia, and Brazil. Across the globe, many countries could potentially recover hydrocarbons from shale reservoirs at large scale. Presently, due to political, environmental, infrastructure and financial constraints only some nations are pursuing the recovery of hydrocarbons from shale at scale, most notably the United States, Argentina and China. In light of recent geopolitical developments (e.g., the Russian invasion of Ukraine), the question remains whether other nations will follow suit and choose to produce oil and gas domestically rather than relying on international partnerships to secure the supply of fossil energy.

As per Sönnichsen (2020), the largest shale oil producers based on daily average crude oil and condensate production in the United States in 2020 were Chevron, EOG Resources, ConocoPhillips & Concho, Occidental Petroleum and ExxonMobil/XTO. In turn, the largest producers of natural gas from shale formations are EQT Corporation, Continental Resources, Marathon Oil, Hess Corporation and Chesapeake Energy Corporation. Notably, the well-established supermajors (i.e., ExxonMobil, Chevron, ConocoPhillips, Shell, BP, Total and Eni) are active shale oil and gas producers, but several smaller and less-known organizations lead the production charts. The major U.S. basins these companies operate in are Anadarko, Appalachia, Bakken, Eagle Ford, Haynesville, Niobrara, and Permian (see Figure 4 below).

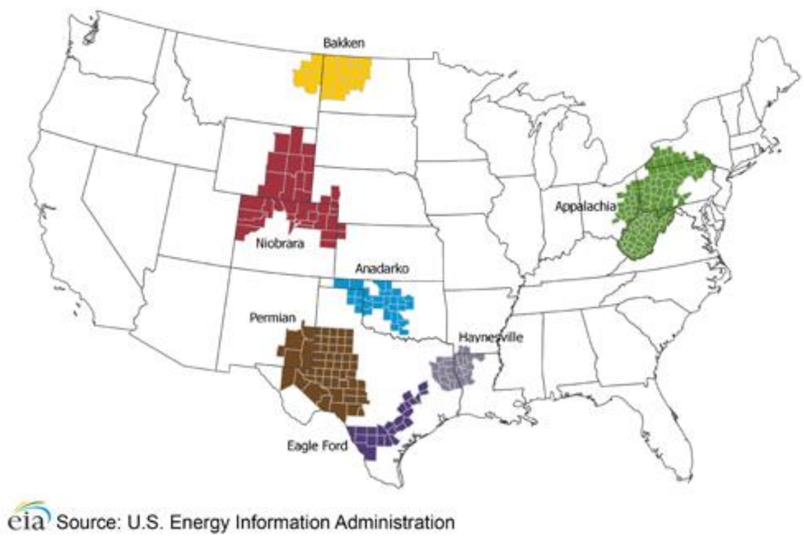


Figure 4: Major shale basins in the United States
(Source: [U.S. Energy Information Administration])

The exploitation of shale resources across the United States has undoubtedly had a dramatic effect on the energy landscape across the globe. In a matter of years, North America went from being an energy importer to one of the largest international exporters of fossil fuels. But access to shale did not only impact the energy industry. As Siirola (2014) points out, it also provided the chemical industry in the United States with a valuable feedstock for petrochemical applications. In 2015, the multinational oil and gas company, Shell, began the construction of a world scale ethylene cracker plant just north of Pittsburgh, Pennsylvania, that will be able to produce over a million tons of plastic pellets per year (Corkery, 2019). Shell's ethylene plant uses as a feedstock ethane from shale gas recovered in the nearby Appalachian Basin.

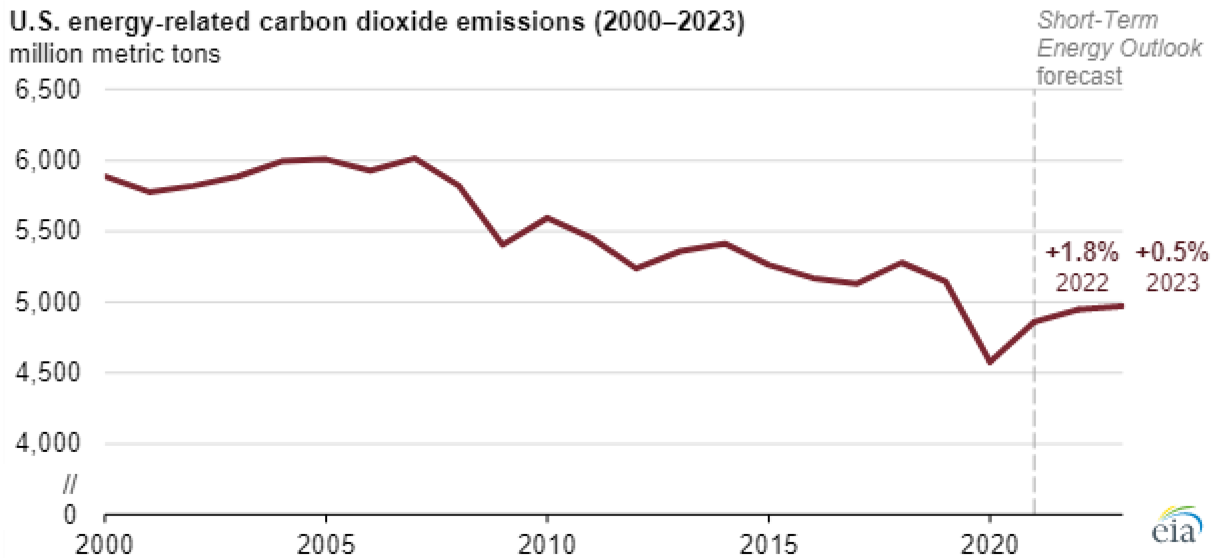


Figure 5. U.S. energy-related carbon dioxide emissions between 2000 to 2021 (Image source: https://www.eia.gov/todayinenergy/detail.php?id=50958)

Finally, it is worth highlighting that ever since shale development activities started ramping up in the United States around 2005, energy-related CO_2 emissions have dropped considerably as shown in Fig. 5. In fact, between 2005 and 2016 alone, emissions fell by 14%. To a large extent, this drop is due to coal being replaced by natural gas for power generation. The implication is that the widespread development of shale resources across the United States – while often perceived as a threat to or burden on the environment – has likely contributed to substantial reductions in energy-related CO_2 emissions in North America in recent history. For regions and countries eager to secure their domestic energy supply while also advancing emission reduction ambitions, the development of shale gas resources, in particular, as a transition step to full carbon neutrality, may be a worthwhile option to consider.

3. Mathematical Programming Models for Shale Development

3.1 Early History of Shale Development Optimization

Seminal contributions presenting optimized strategies to exploit shale deposits started in the 1970's (Crookston, 1975). The first studies assessed pyrolysis as an alternative technology for oil extraction (Wen & Yen, 1977; Gurfel, 1979). In the 1980's, the first optimization techniques to better fracture shale formations with different fluids, including brine and CO_2 mixtures, came to light (Bonse, 1980; Swartz, 1982). Production optimization in shale wells was addressed by Reeves, Hill & Cox in 1993, while the earliest contributions to the design of shale well fractures accounting for life cycle, water usage and environmental considerations were proposed in 2008

(Miskimins, 2008; Gaudlip et al., 2008). By that time, contributions in the field were merely 10% of the total number of works that we find nowadays, and most of them dealt with shale oil production. The number increases to 25% as of 2014, now including deeper analysis on the economic and environmental impact of shale gas production (Stephen, 2010; Jiang et al. 2011; Guarnone et al., 2012). Cafaro & Grossmann (2014) developed the first optimization model on the strategic planning, design, and development of the shale gas supply chain. Since then, the number of contributions to the field has increased steadily.

In 2017, Gao & You (2017) published the first and most recent review of publications concerned with the design and optimization of shale energy systems. The review was limited to research on shale gas only. This review considers all work related to the optimization of shale oil and gas resources since 2017. Nearly half of all publications on shale oil and gas development optimization have appeared since that time. Also, recent geopolitical events (i.e., the COVID-19 pandemic, the Russian invasion of Ukraine) have sparked debate among the academic community and the general public, on the importance and implications of hydrocarbon recovery from shale resources across the world.

3.2 Major Topic Areas

As part of this review, we distinguish between five major topics areas in the field of shale oil and gas optimization, as shown in Fig. 6, namely: (1) development planning, (2) production optimization, (3) supplies, gathering & processing optimization, (4) water management, and (5) life cycle analysis (LCA) & sustainability.

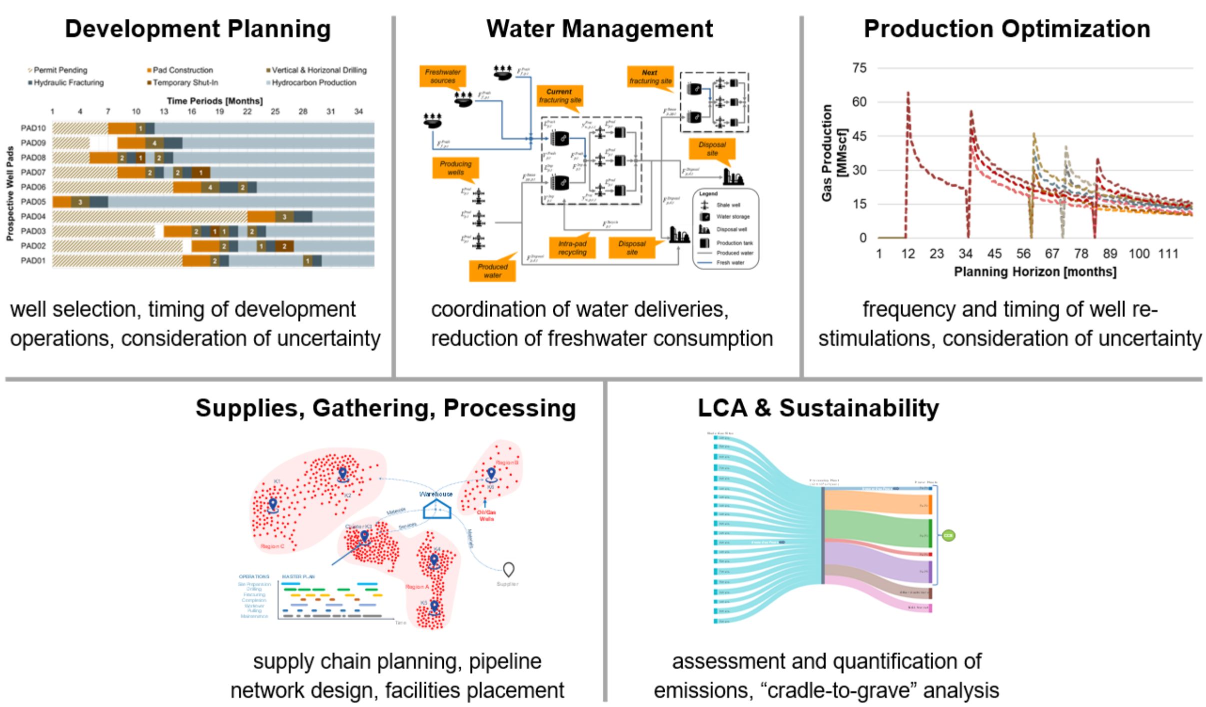


Figure 6. Main topic areas in the field of shale oil & gas optimization

Development planning describes activities associated with the scheduling and planning of shale drilling, fracturing and production operations. Researchers active in this space put forward mathematical programming models to help decision-makers understand where to focus and how to coordinate development activities so as to improve economic or environmental objectives.

The **production optimization** topic area, on the other hand, is concerned with how to maximize the recovery of hydrocarbons from shale reservoirs. The manipulation or coordinated control of production parameters (e.g., well head pressure or artificial lift systems) can greatly improve well economics at moderate expense. In turn, some researchers have studied whether and how upstream production control strategies can be leveraged to optimally respond to downstream demand changes (e.g., natural gas power plants).

Work on **supplies, gathering and processing optimization** has been equally prominent over the past years. It should be noted that this field of study is closely related to development planning – for good reason. For instance, the timing of drilling and completions operations drives the construction of midstream oil and gas gathering infrastructure. However, the opposite is true as well. Neither oil nor gas produced from shale reservoirs can be recovered at scale if the respective pipelines and/or processing facilities have not been constructed on time and sized appropriately. The distinguishing characteristic is that development planning is an activity usually carried out by upstream operators only, whereas supplies, gathering and processing optimization primarily falls onto service companies and mid-/ downstream entities.

Water management is essential to shale oil and gas development. For one, it is well-known that the extraction of hydrocarbons from unconventional reservoirs is very water-intensive. At the same time, the production of oil and gas from shale formations is generally accompanied with water, adequately referred to as "produced water". Upstream companies need to manage both: supply and demand. Sufficient water needs to be sourced and transported to a well site prior to and during hydraulic fracturing operations – which can be a logistical challenge in and of itself. But then, post-completions, substantial quantities of produced water are brought to the surface and must be transported off-site to maintain hydrocarbon flow. The management of water is arguably one of the most challenging, yet underappreciated aspects of unconventional development.

Finally, we introduce a topic area dedicated to **LCA and sustainability**. Shale oil and gas development – but hydraulic fracturing in particular – is a controversial topic among scholars and the general public alike. The significant water demand, the potential contamination of water sources, the potential release of greenhouse gas (e.g., methane) emissions, the association with induced seismicity (i.e., earthquakes), the safety of pipelines – and general concerns regarding the need for fossil fuels – have been and continue to be contested points of debate. Not surprisingly, the academic community has responded by proposing optimization tools to quantify and assess the environmental performance of shale oil and gas development. Life cycle analysis has emerged as a powerful and insightful framework to better understand "cradle-to-grave" implications of hydrocarbon recovery from shale reservoirs (Chen et al., 2019). Many important contributions over the past few years fall into this very topic area.

While some work over the past years has attempted to holistically study shale oil and gas optimization opportunities across all of these domains, most publications can be attributed to one of these five topic areas. However, one other distinguishing feature of publications in this space is the spatial scope of work in the field, ranging from: (1) a single shale oil or gas well, (2) a multi-well pad, (3) a development or gathering system comprised of multiple well pads within a contiguous geographical area, (4) multiple disjoint gathering systems managed by a single entity, and (5) the national scale.

For a detailed breakdown of publications by topic areas and scope, we refer to Table 1. As can be seen from the table, most research to date has been focused on individual development areas or systems, especially work related to water management and development planning. Not surprisingly though, studies concerned with life cycle assessments, or the general sustainability of shale oil and gas development activities frequently tend to consider a broader scope. At the extreme ends of the spectrum, very few publications have been concerned with the optimization of individuals wells, or development activities at the national scale. This is somewhat surprising given that both fields of study – the smallest functional unit of a development program (i.e., a well) up to the nationwide perspective – would likely benefit the academic community in pursuing optimization opportunities. Interestingly, in their 2017 review, Gao & You (2017) highlighted a dozen publications that were concerned with the design and operation of shale gas energy systems at either the national or even global scale.

	Single Well	Multi-Well Pad	Single System	Multiple Systems	National Scale
Development Planning		Ondeck et al. (2019a), Li et al. (2020)	Gao et al. (2018), Peng et al. (2020), Bean (2020), Peng et al. (2021), Soni et al. (2021), Díaz-Gómez et al. (2021)	Ondeck et al. (2019b)	
Production Optimization	Drouven et al. (2017), Cafaro et al. (2018), Zuo & Cremaschi (2021)	Hülse et al. (2020), Calderón & Pekney (2020), Achkar et al. (2021)	Foss et al. (2018)		
Supplies, Gathering, Processing Optimization			Drouven & Grossmann (2017), Hong, Li, Song et al. (2020), Allen et al. (2019)	Montagna & Cafaro (2019), Hong, Li, Di et al. (2020)	Tan & Barton (2017)
Water Management			Drouven & Grossmann (2017), López-Díaz et al. (2018), Tavakkoli (2018), Carrero-Parreño et al. (2018), Ahmad et al. (2019), Carrero-Parreño et al. (2019), Al-Aboosi & El-Halwagi (2019), Ren et al. (2019), Cafaro & Grossmann (2020)	Oke et al. (2019), Oke et al. (2020)	
Life Cycle Analysis & Sustainability			Wang & Zhan (2019), Kroetz et al. (2019), Caballero et al. (2020)	Gao & You (2017a), Gao & You (2017b), Gao & You (2018), Gao (2018), Gao & You (2019), Chen et al. (2017),Chen et al. (2018)	

Table 1: A summary of publications related to shale optimization since 2017 by topic areas and scope

Figure 7 shows publications related to shale oil and gas optimization by topic areas over the years. Even though this review focuses on work after 2017, we include here all optimization-based contributions considered by Gao & You (2017). We attribute pre-2017 publications to topic areas as follows:

- Development planning: Cafaro & Grossmann (2014), Calderón et al. (2015a), Calderon et al. (2015b), Gao and You (2015a), Arredondo-Ramirez et al. (2016), Drouven & Grossmann (2016), Guerra et al. (2016)
- Production optimization: Knudsen & Foss (2013), Knudsen et al. (2014a), Knudsen et al. (2014b), Knudsen & Foss (2015), Cafaro et al. (2016)
- Supplies, gathering and processing: Martin and Grossmann (2013), Wang et al. (2013), Noureldin et al. (2014), Wang and Xu (2014)
- Water management: Yang et al. (2014), Yang et al. (2015), Gao and You (2015b), Bartholomew and Mauter (2016), Lira-Barragán et al. (2016)
- LCA & sustainability: Gao and You (2015c), Pascual-Gonzalez et al. (2016)

Figure 7 below considers all publications captured in Table 1, as well as the contributions listed above.

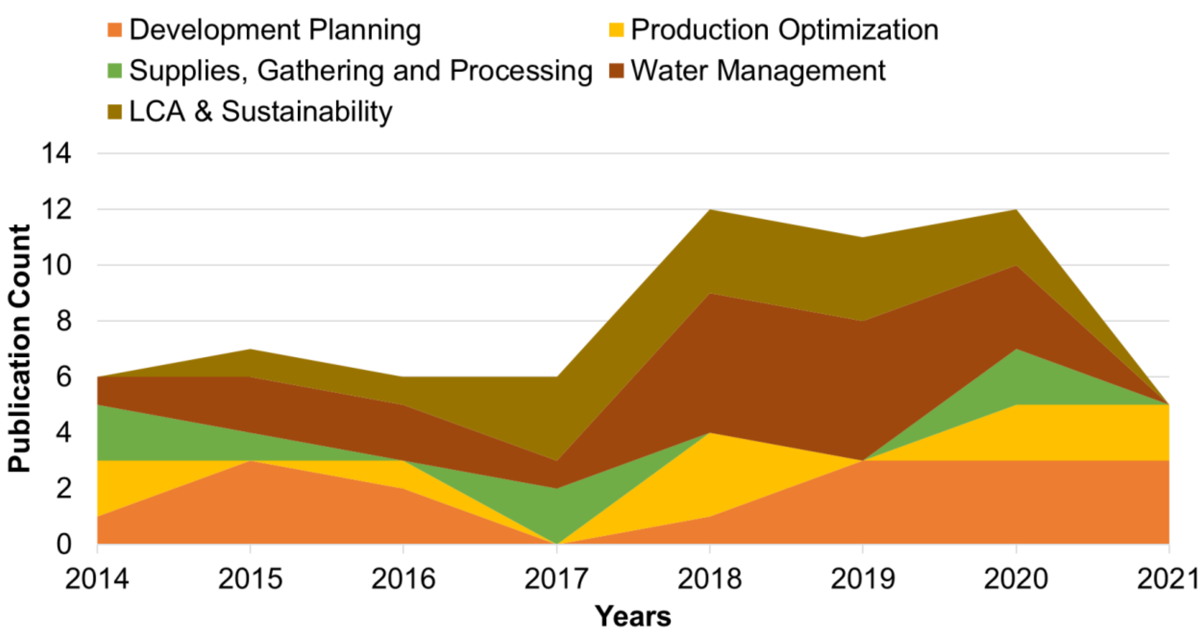


Figure 7: Publication count by topic areas since 2014

3.3 Development Planning

At its core, development planning optimization models are meant to help upstream organizations identify feasible and economically attractive drilling, fracturing and production schedules. At the onset of the “shale revolution”, this task seemed reasonably straightforward. Companies would move drilling rigs and fracturing crews to suitable well pads, and then drill and complete as many wells as they could. Over time, though, researchers and the industry realized that this approach was oftentimes suboptimal since it could take months before production would start, leading to delayed returns on investment. The realization that drilling and fracturing schedules were powerful degrees of freedom, opened the door for leveraging mathematical programming for decision-support. The underlying scheduling and planning problems are inherently discrete in nature since it is neither practical nor desirable to drill or complete fractional wells. Companies must commit to development decisions months if not years in advance, and the timing of upstream decisions has to be closely coordinated with midstream activities (i.e., construction and/or operation of pipelines) to prevent costly inefficiencies.

As illustrated in Table 1, the scope for development planning optimization can range from individual multi-well pads (Ondeck et al., 2019a, Li et al., 2020) to single systems containing multiple pads (Gao et al., 2018, Peng et al., 2020, Peng et al., 2021, Soni et al., 2021, Díaz-Gómez et al., 2021, Bean, 2020) to multiple systems across geographically distributed areas (Ondeck et al., 2019b). Nearly all publications in recent years are geared at planning horizons spanning multiple years. Discrete-time formulations are predominant with planning horizons being discretized by either weeks, months, annual quarters or even years.

Since the pioneering work on development planning optimization by Cafaro & Grossmann (2014), this topic area continues to receive a considerable amount of attention by the academic community. Virtually all contributions in recent years have been mixed-integer linear and nonlinear programming models. Discrete and/or integer variables are introduced to capture decisions related to scheduling of drilling/fracturing activities, or the existence/placement/sizing of supporting and midstream infrastructure (i.e., pipelines, compressor stations, water storage or treatment facilities and processing or power plants). Fig. 8 shows a representative development schedule, illustrating the complexity involved in development planning problems.

Annual Quarters

Pad	Operation	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
A1	TS										14		10					13	20									12			
A1	HZ										14			10					21	11								12			
A1	FRAC											14		10					12		10	10	10					12			
A1	TIL											14		10					12		10	10	10					12			
A2	TS	21	14				11						18		19					13		30	10		14						
A2	HZ	21	14					11					12		25					13		12	29		14						
A2	FRAC	21	14					11					12		12	13					11	14	14	15	14						
A2	TIL		35						11				12		12	13					11	14	14	15	14						
B1	TS					18	19		37								13							21			34				
B1	HZ					10	17	10		15		22					13							21			22				
B1	FRAC						25	13		15		22					13							10		11			10		
B1	TIL						18	19		15		12	10				13							10		11			10		
B2	TS			10							12				10					10		20								17	
B2	HZ				10						12				10					10		20								17	
B2	FRAC				10							12			10					17					10	10				17	
B2	TIL				10							12			10					17					10	10				17	
C1	TS							10	10	14	21			12							13	16									
C2	HZ								15	19				33							13	16					12				
C3	FRAC								11	12	11			11	11	11					13	16					12				
C4	TIL								11	12	11			11	11	11					13	16					12				

Fig. 8. Development schedule for a shale gas field illustrating the combinatorial complexity of the underlying development planning problem (Note: development pace indicated in thousands of "feet-of-pay" (i.e., combined lateral length) where TS = top-setting, HZ= horizontal drilling, FRAC=hydraulic fracturing, and TIL=turning in line) [adapted from Ondeck et al., 2019b].

Originally, researchers proposed mixed-integer nonlinear programs to consider economies of scale for sizing supporting infrastructure (e.g., compressor stations, pipelines, processing plants) or for addressing variations in the composition of the hydrocarbons extracted (Drouven & Grossmann, 2016). More recently, however, the community appears to have been gravitating towards larger yet predominantly mixed-integer linear programs. Additional complexity is introduced by considering uncertainty in the planning process. Uncertain parameters include the expected ultimate recovery (EUR), production rates (Gao et al., 2018; Peng et al., 2021) and commodity prices (Li et al., 2020; Bean, 2020).

Also, researchers are now increasingly acknowledging that it can be beneficial or even necessary to consider the fact that drilling and fracturing operations require different types of resources. As discussed earlier, the vertical section of a shale well is generally drilled with a so-called "topsetting" rig whereas the lateral section of the well requires a "horizontal" rig. Hydraulic fracturing of the wells itself is performed by a fleet of trucks equipped with high-pressure pumps. Since assembling and dissembling these rigs and their respective crews is not an easy undertaking, several recent publications (Ondeck et al., 2019a, Ondeck et al., 2019b) have proposed mathematical programs that account for the respective resource movements and mobilization costs (which can amount to several hundreds of thousands of dollars per rig/crew).

It should also be noted that out of the eleven publications identified in Table 2, only one is concerned with shale oil development (Soni et al., 2021). All other publications address shale gas development problems. Although the development process is similar for both, oil produced from shale formations tends to require more upstream processing (e.g., fluids separation) which adds to the complexity of the development process. Also, the economic impact of oil recovery projects tends to be much more significant than for gas projects. Finally, we note that the predominant objective for development planning optimization is to maximize the net present value (NPV) of the upstream endeavor, which is not surprising given the capital-intense nature of oil and gas development projects, the extended planning horizons, and a focus on maximizing production-related revenues. Given that production volumes are directly tied to the development schedule, as illustrated in Fig. 9, development planning is of significant importance to the economic performance of any upstream organization.

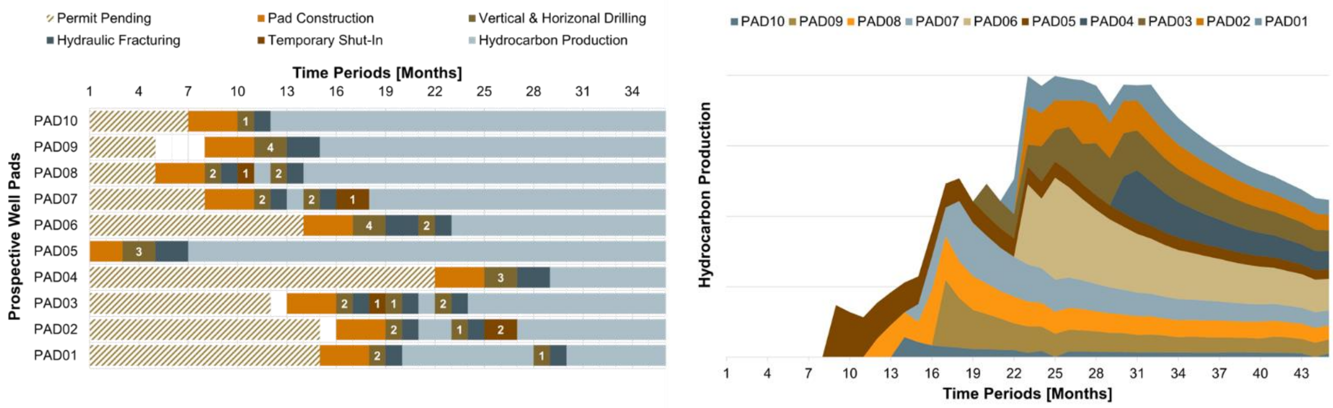


Fig. 9. Development strategy and corresponding production profile (adapted from Drouven & Grossmann 2016)

Publication	Oil/Gas	Problem Scope	Objective(s)	Degrees of Freedom	Model Type	Solution Strategy	Uncertainty Consideration
Cafaro & Grossmann (2014)	Gas	Upstream & midstream	Max NPV	Drilling schedule, processing plant placement/sizing, pipeline routing/sizing, compressor placement/sizing	MINLP	Custom branch-and-refine decomposition strategy	No
Drouven & Grossmann (2016)	Gas	Upstream & midstream	Max NPV	Drilling & fracturing schedule, pipeline routing/sizing, compressor placement/sizing, midstream agreement selection	MINLP	Custom decomposition strategy	No
Gao, Ning & You (2018)	Gas	Upstream, midstream & downstream	Min costs	Drilling schedule, processing plant placement/sizing, pipeline routing/sizing	MILP	Reformulation	Yes (EUR and market demand)
Ondeck et al. (2019a)	Gas	Upstream	Max profit	Drilling, fracturing and production schedule, development resource allocation	MILP	Commercial solver	No
Ondeck et al. (2019b)	Gas	Upstream & midstream	Max NPV	Drilling, fracturing and production schedule, resource allocation	MILP	Commercial solver	No
Li et al. (2020)	Gas	Upstream	Max NPV	Drilling, fracturing, and production schedule	MILP	Commercial solver	Yes (Price forecasting)
Peng et al. (2020)	Gas	Upstream & midstream	Max NPV	Drilling, fracturing and production schedule	MILP	Bilevel decomposition algorithm	No
Peng et al. (2021)	Gas	Upstream & midstream	Max NPV	Drilling, fracturing and production schedule	MILP	Langrangean decomposition algorithm	Yes (Production uncertainty)
Soni et al. (2021)	Oil	Upstream & midstream	Max NPV	Drilling and fracturing schedule	MILP	Rolling horizon approach	No
Díaz-Gómez et al. (2021)	Gas	Downstream	Max NPV	Design of integration production network	MILP	Commercial solver	No
Bean (2020)	Gas	Downstream	Max NPV	Gas production	MILP	Commercial solver	Yes (Price forecasting)

Table 2: Detailed comparison of selected, recent publications on shale development planning optimization

3.4 Production Optimization

Production optimization models in the shale oil and gas industry involve a series of strategies to sustain or improve well productivity over longer time horizons, oftentimes extending their economic lifespan. This is certainly critical for the operation of unconventional wells due to the steep declines that characterize shale oil and gas productivity. Attempts to optimize the productivity of shale wells can be roughly categorized into four groups, in ascending order of complexity from an operational viewpoint: choking and shut-ins, artificial lift, refracturing and enhanced-oil-recovery.

3.4.1. Choking and Shut-ins

Foss et al. (2018) introduce the concept of daily production optimization (DPO) problems in which production engineers aim to utilize the production systems as efficiently as possible. This is done by adjusting control inputs like choke valves. They present a discussion on appropriate formulations, in particular the use of static models vs. dynamic models, to address these problems.

Many important problems can indeed be solved by repetitive use of static models while some others, in particular related to shale gas systems, require dynamic models to capture key process characteristics. The work in this field highlights that daily production optimization problems are well suited for mathematical optimization. Foss et al. (2018) propose a Generalized Disjunctive Programming (GDP) model and MINLP reformulations to solve a dynamic optimization framework based on proxy reservoir models. A receding horizon optimization strategy is repetitively solved at each time step. On the other hand, whenever reservoir dynamics can reasonably be neglected, a static model is proposed for each time step. Piecewise linear approximations are used to convert the MINLP into an MILP. From simulation analysis, it is argued that a static optimization formulation suffices in most relevant DPO cases, in particular for oil production from offshore well platforms. Important exceptions are shale gas wells and thin oil rims.

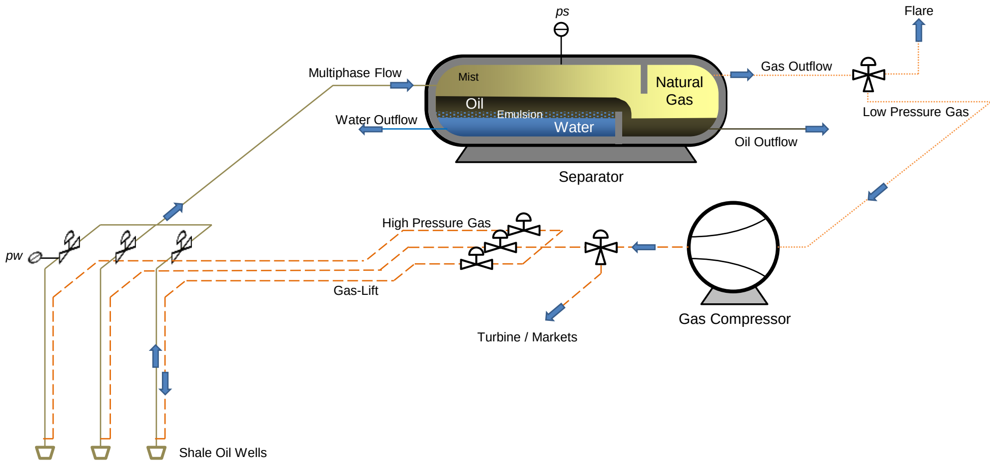


Fig 10. Simplified illustration of an oil production platform or well pad, with gas-lift operations (adapted from Hulse et al., 2020)

Hulse et al. (2020) suggest that static models are applicable when the optimization time-scales are faster than the underlying reservoir dynamics, and slower than the dynamics of top-side equipment. Fig. 10 illustrates an oil production platform with valves for choking wells and compressors for gas-lift operations. Essentially, static problems are effectively solved over time in response to changes in the prevailing conditions, which will remain persistent for long periods. However, when surface conditions change frequently or suddenly - potentially due to reduced processing capacity – it is argued that the dynamics of wells should not be neglected and well operations should be scheduled over time (specifically when wells are shut-in due to processing capacity drops and restarted later as the normal conditions are recovered). By modeling the approximate dynamics of well startup, these optimization models seek to find the best operations schedule of a platform or well pad when some wells are shut-in and restarted due to varying compression capacity. It is clear that better results can be achieved when the methodology is supported by more accurate simulation models and systems parameters. Nevertheless, given the large number of decisions involved in this kind of problem, even for small instances (with few wells and time steps), it is still an open question to what extent it is worth including more details (thus adding more complexity) into the decision-making tool.

3.4.2 Artificial lift

Artificial lift methods or systems involve a wide range of techniques aimed at deliquefying shale gas wells. Although these operations are relatively mature for vertical wells in conventional reservoirs, enhancing the productivity of horizontal shale oil and gas wells has become a new frontier for unconventional production. An artificial lift infrastructure plan includes the selection of appropriate equipment and its operating schedule. This problem was first addressed by Zuo and Cremaschi (2018), and later extended by the same authors (Zuo and Cremaschi, 2021). The authors propose a discrete-time MINLP model to solve a multistage stochastic formulation. They incorporate endogenous uncertainty in the well response, and exogenous uncertainty in shale gas prices, although the latter uncertainty does not seem to affect the optimal solutions. The models are tested for two case studies that utilize the production history of two wells in the Woodford Play (US). Although the models consider the possibility of multiple artificial lift methods (i.e., ALMs), the scope is limited to the lifespan of a single well. Achkar et al. (2021) develop an extended MILP formulation determining the integrated planning of several artificial lift systems in a multi-well pad. The model simultaneously manages ALM selection, investment and operational decisions, introducing very detailed piecewise functions accounting for installation and disassembly times. As in every discrete-time approach, the major limitation is the size of the MILP model, even under the assumption that the well response and the gas prices are given data (deterministic models). The authors conclude that the number of resources (i.e., ALM) seems to have a higher impact than increasing the number of wells in the pad.

3.4.3 Refracturing

Refracturing presents a promising strategy for addressing the characteristically steep decline rates of shale wells. The core idea behind refracturing is to restimulate the reservoir such that it yields previously untapped hydrocarbons and improves the overall production profile of a well. The seminal work on the optimal planning refracture treatments on shale gas wells was proposed by Drouven, Cafaro and Grossmann (2016). They present both a continuous time nonlinear programming (NLP) model based on a novel forecast function that predicts pre- and post-treatment productivity declines, and a discrete-time, multi-period MILP model that explicitly accounts for the possibility of multiple refracture treatments over the lifespan of a well. The NLP model was extended to account for multiple refractures along the lifespan of the well (Cafaro et al., 2018), also considering the calculation of the net present value (NPV) of the project over continuous time domains.

For the discrete-time model, three alternative reformulations from the same disjunctive program are compared against each other (big-M, Standard and Compact Convex-Hull). The proposed framework is limited to a single well and can be applied to either new or existing wells, to determine whether or not refracture treatments make economic sense. The optimal number of refracture treatments and their timing are highly sensitive to the underlying natural gas price forecast. That is why two years later, the same authors extend their model to address exogenous price forecast uncertainty together with endogenous uncertainty associated with the well response to refractures (Drouven et al., 2017). A two-stage MILP stochastic programming model embedded in a moving horizon strategy is developed to dynamically solve the planning problem under endogenous uncertainties. A generalized production estimate function predicts the gas production over time depending on how often a well has been refractured, and when exactly it was restimulated last. From a detailed case study, it is concluded that early in the life of an active shale well, refracturing makes economic sense even in low-price environments, whereas additional restimulations only appear to be justified if prices are high (see Fig. 10). The model is still limited to a single well.

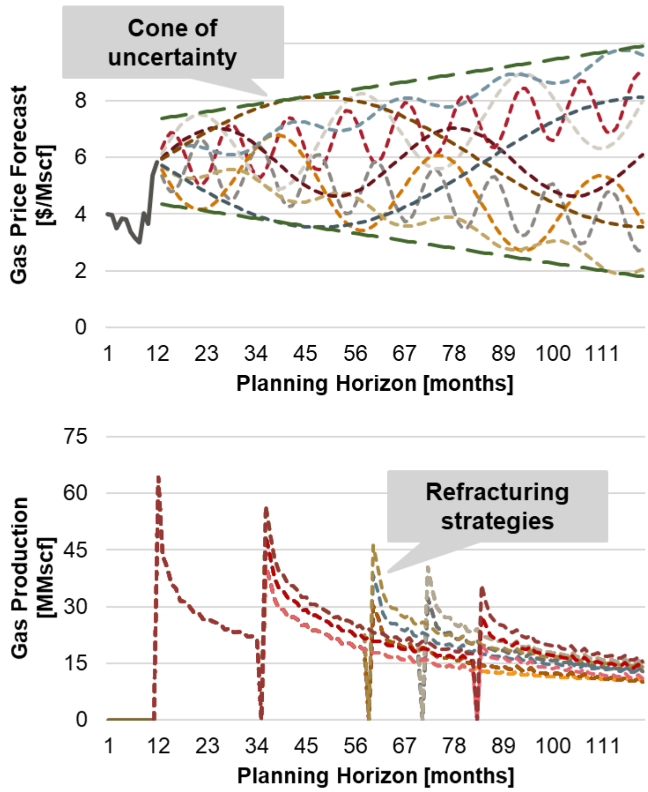


Fig. 11: Representative illustration of optimization-based refracturing planning in light of uncertain gas price forecasts (i.e., cone of price uncertainty) and uncertain post-refracture production performance (adapted from Drouven et al., 2017)

3.4.5 Enhanced-oil-recovery (EOR)

In recent years, technologies that tackle gas flaring activity in oil production have been a focal point. One of the promising alternatives is the injection of flare gas into the reservoir to stimulate production of shale oil and capture associated natural gas. Calderon and Pekney (2020) address the optimal planning of EOR in shale oil development to reduce gas flaring. A multiperiod MINLP framework optimizes decisions such as drilling schemes, workover of depleted production wells, pipeline and processing infrastructure, placement of injection sites, injection rates, and duration of EOR operations. Due to the complexity of the mathematical model, a heuristic strategy is proposed to overcome convergence issues. The authors propose to solve a sequence of static optimization models, then refined by pseudo-dynamic models that include surrogate functions to approximate the transients. Piecewise linear approximations are finally used to linearize the MINLP model. They conclude that EOR greatly favors the economics and contributes to the reduction of gas flaring, but it is insufficient to comply with flaring targets imposed for the Bakken shale.

Publication	Oil/Gas	Problem Scope	Objective(s)	Degrees of Freedom	Model Type	Solution Strategy	Uncertainty Consideration
Drouven et al. (2016)	Gas	Upstream	Max EUR / Max NPV	Refracturing timing	NLP, MILP	Reformulations of Disjunctive Programming Models.	No
Drouven et al. (2017)	Gas	Upstream & Midstream	Max NPV	Decisions to drill, refracture or wait (here-and-now) + Recourse actions (drill, (re)refracture or wait).	MILP	Two-stage stochastic programming over a moving-horizon framework.	Yes (exogenous: gas price, endogenous: well productivity/ response)
Cafaro et al. (2018)	Gas	Upstream	Max EUR / Max NPV	Refracturing timing	NLP	Global optimization solver.	No
Zuo & Cremaschi (2021)	Gas	Upstream	Max NPV	Selection of artificial-lift system. Time to install and remove ALS.	MINLP	Multi-stage stochastic programming.	Yes (exogenous: gas price, endogenous: ALS productivity)
Achkar et al. (2021)	Gas	Upstream	Max NPV	Selection of artificial-lift systems. Allocation to wells. Time and length of lifting.	MILP	Commercial solver	No
Hülse et al. (2020)	Oil & Gas	Upstream	Max NPV	Well shut-ins and restart operation times. States and control variables.	Pseudo-dynamic models + MILP	Decomposition (sequential) – Piecewise linear approx.	No
Calderón & Pekney (2020)	Oil & Gas	Upstream	Max NPV	Drilling (production & injection wells) + conversion. Facilities installation. Recycling and flaring.	MILP	Iterative cluster-based strategy.	No (just a sensitivity analysis)
Foss et al. (2018)	Oil / Gas	Upstream & Downstream	Max NPV	Well shut-ins and routing decisions. States and control variables.	GDP	MINLP reformulation	No

Table 3: Detailed comparison of selected, recent publications on shale production optimization

3.5 Water Management

Water management is an important, complex, and cost-intensive aspect of shale oil and gas development. The extraction of hydrocarbons from unconventional reservoirs requires very large quantities of water. Drilling and hydraulically fracturing a single shale well can consume over a million barrels of water – which is the equivalent to about 63 Olympic-size swimming pools. However, companies rarely complete just one well at a time. Nowadays, multiple wells are fractured in parallel or in sequence at one well site. Up to 70 wells can originate from one well pad, suggesting that the overall demand for water at one given location can be tens of millions of barrels. At the same time, shale oil and gas wells produce significant quantities of high-TDS water along with hydrocarbons. Due to its salinity, this so-called produced water can generally not be released into the surface environment. Produced water is commonly either injected underground for disposal purposes or reused by the oil and gas industry to meet the water demand for subsequent drilling and fracturing operations. Actual desalination of produced water continues to be rare and is usually limited to niche applications.

Shale water management optimization continues to be an active area of research. Over the years, there has been a consistent stream of publications in this space, as shown in Fig. 7. Nearly all work has been concerned with the management of water (i.e., balancing of supply and demand). Notably, not a single publication to date has focused on the management of water specifically for shale oil systems. Several relevant publications in this area co-optimize shale water management operations along with fracturing schedules – which drive both water demand but also water supply (i.e., flowback) post-production. Given that the fracturing schedule decisively sets the oil and gas production schedules, several researchers choose the maximization of profits or NPV as their preferred objective function. The idea is to find ways to accelerate the onset of oil or gas production revenues while minimizing the costs of managing water. It should also be noted that setting the fracturing schedule involves inherently discrete decisions (i.e., the sequencing of well development operations). This partially explains why mixed-integer programming models are so prevalent in this area.

The major degrees of freedom in shale water management optimization are: (1) where to source water from to support completions operations (i.e., fresh/brackish or produced water sources), (2) where to deliver produced water to (i.e., disposal facilities, completions sites or treatment centers), and (3) which type of supporting infrastructure to leverage (i.e., pipelines, storage units, treatment facilities, injection wells). Fig. 12 shows a summary of common shale water management options. The latter generally involves the selection of discrete sizes of standardized equipment, which adds binary and integer variables to mathematical programming formulations. Very few publications to date have explicitly considered water quality as part of the water management optimization framework; with work by Yang et al. (2015), Guerra et al. (2016) and Carrero-Parreño et al. (2018) being the exceptions.

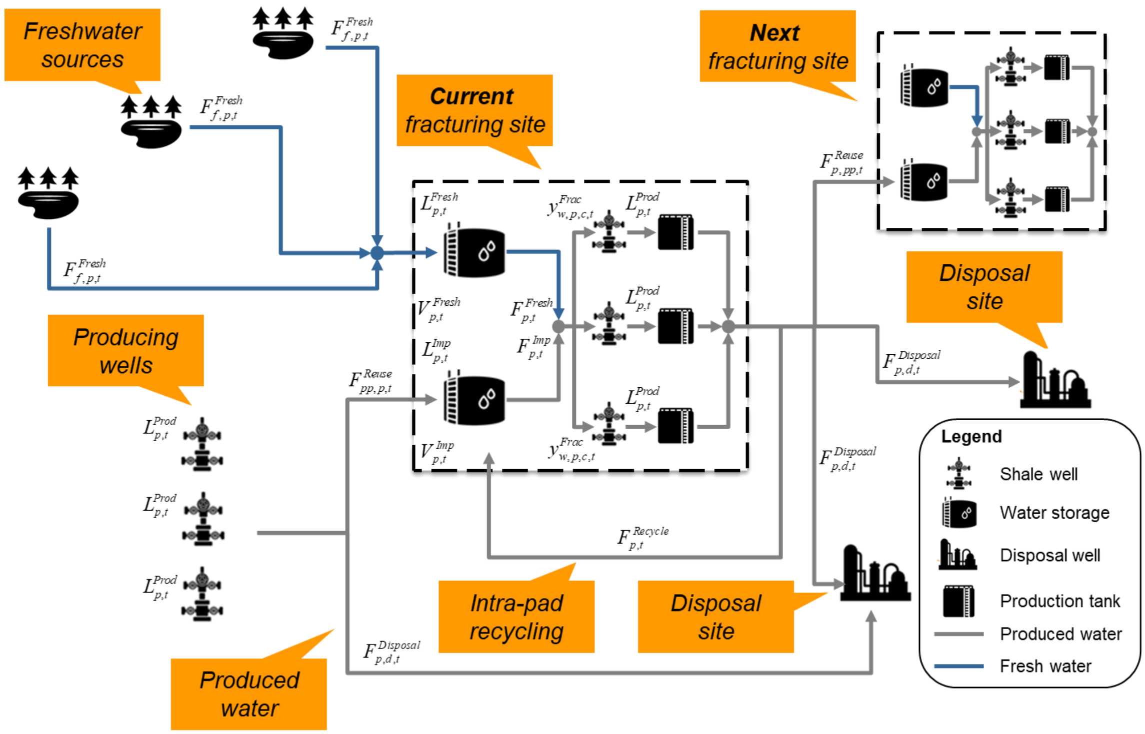


Figure 12. Superstructure illustration of water management operations in shale plays (adapted from Drouven & Grossmann 2017)

Aside from Ren et al. (2019), all relevant publications since 2017 propose mixed-integer programming models. The majority of these are mixed-integer linear programs. When nonlinearities are introduced, the respective models consider changes in water quality, i.e., bilinear terms as the result of multiplying unknown flows with unknown concentrations (Carrero-Parreño et al., 2018) or they capture economies of scale, i.e., power law functions (López-Díaz et al., 2018; Tavakkoli 2018). In this context, it is worth noting that to date there has been little work on developing custom solutions algorithms for mathematical programming models addressing shale water management. Most researchers rely on commercial solvers (e.g., CPLEX or Gurobi) to solve the respective optimization problems.

Finally, we draw attention to the fact that few publications related to shale water management optimization have explicitly considered uncertainty in model parameters. When stochastic programs have been proposed, they were accounting for uncertain water availability (Yang & Grossmann, 2014), hard-to-predict water demand and flowback volumes (Lira-Barragán et al., 2016), or unknown gas prices and demands (Oke, 2020). Although not technically dealing with uncertainty, the work by Carrero-Parreño et al. (2019) stands out for focusing on quantifying the benefits of multiple entities managing, and potentially sharing, water within an active development area.

Publication	Oil/Gas	Problem Scope	Objective(s)	Degrees of Freedom	Model Type	Solution Strategy	Uncertainty Consideration
Drouven & Grossmann (2017)	Gas	Water management	Max NPV	Fracturing schedule, produced water deliveries, water blending, storage placement/sizing	MILP	Commercial solver	No
López-Díaz et al. (2018)	Gas	Water management	Min costs, environmental impact	Count/sizing of storage/treatment units/disposal sites	MINLP	Commercial solver	No
Carrero-Parreño et al. (2018)	Gas	Water management	Max sustainability profit	Freshwater sourcing, placement/sizing storage tanks, drilling/fracturing schedule, water reuse, treatment facilities	MINLP	Custom decomposition strategy	No
Tavakkoli (2018)	Gas	Water management	Min costs	Coordination of water transportation/treatment/disposal, sizing/placement of treatment units	(MIN)LP	Genetic algorithm	No
Ahmad et al. (2019)	Gas	Water management	Min costs	Freshwater sourcing, disposal volumes, treatment/disposal capacity expansion	MINLP	Commercial solvers	No
Carrero-Parreño et al. (2019)	Gas	Water management	Max coalition profit	Water sourcing, placement/sizing storage tanks, drilling/fracturing schedule, operator payoffs	MILP	Commercial solver	No
Al-Aboosi & el-Halwagi (2019)	Oil & gas	Produced water treatment	Max profit	Treatment design parameters	MINLP	Commercial solver	Yes (Solar irradiance, fuel price)
Oke et al. (2019)	Gas	Upstream, midstream, downstream and water management	Max profit	Water sourcing, fracturing schedule, water treatment design, sizing of processing/power plants/pipelines	MINLP	Commercial solver	No
Ren et al. (2019)	Gas	Water management	Min costs, freshwater use	Water coordination (i.e., freshwater, flowback/produced water)	LP	Compromise programming	Partial (Sensitivity analysis)
Cafaro & Grossmann (2020)	Gas	Upstream development planning and water management	Max NPV	Size/placement of water pipelines and storage facilities, development schedule	MILP	Commercial solver	No
Oke et al. (2020)	Gas	Upstream, midstream, downstream and water management	Max profit	Supply chain network design (including fracturing schedule)	MIP	Commercial solver	Yes (Gas price and demand)

Table 4: Detailed comparison of selected, recent publications on water management optimization

Publication	Oil/Gas	Problem Scope	Objective(s)	Degrees of Freedom	Model Type	Solution Strategy	Uncertainty Consideration
Tan & Barton (2016)	Gas	Upstream & Midstream	Max NPV	Allocation of mobile gas-to-liquids and LNG plants	MILP	Deterministic equivalent of two-stage stochastic programming model.	Yes (exogenous: supply, demand, gas price)
Allen, Allaire, & El-Halwagi (2019)	Gas	Upstream	Min Net Present Cost (NPC)	Number, size, technology and location/allocation of modular gas processing units (skids).	MILP	Deterministic equivalent of a multi-stage stochastic programming model. Superstructure of multidimensional nodes.	Yes (exogenous: production forecast)
Hong, Li, Song, Chen, Zhao & Gong (2020)	Gas	Upstream & Midstream	Max NPV	Production start times. Allocation (purchase and mobilization) of modular gas processing facilities.	MILP	Commercial solver.	No
Drouven & Grossmann (2017)	Gas	Upstream	Max NPV	Wells to turn-in-line. Pressures at the nodes of the pipeline network, flows and compression power to use.	MINLP	NLP for initialization. MILP for bounding. Local MINLP for wells planning. Global MINLP from incumbent.	No
Hong, Li, Di, Song, Yu, Chen, Li & Gong (2020)	Gas	Upstream	Min NPC	Pipeline layouts, connections, diameters and expansions. Flows and pressures over time.	MINLP	Piecewise linear approximation based on discrete ranges for flowrates.	No
Montagna, Cafaro, Grossmann, Burch, Shao, Wu & Furman (2021)	Oil & Gas	Upstream	Min NPC	Number, size and location of tank batteries and processing facilities. Pipeline diameters and connections.	MINLP	NLP-MILP decomposition and refinement strategies for feasible solutions. MILP relaxations for bounds.	No
Tan & Barton (2017)	Oil & Gas	Upstream, Midstream & Downstream (Country-wide)	Max NPV	Location and capacity of plants (refineries, gas-to-liquids and LNG plants).Transportation modes (pipeline, road, rail, barge).	MILP	Deterministic equivalent of two-stage stochastic programming model.	Yes (exogenous: GDP, oil price –gas price linked)
Montagna & Cafaro (2019)	Oil & Gas	Upstream	Min NPC	Location and size of storage facilities. Material and service provision (flows) to wellpads.	MILP	Clustering of wells and locations.	No

Table 5: Detailed comparison of selected, recent publications on supplies, gathering and processing optimization for shale production

3.6 Supplies, Gathering & Processing Optimization

For decades, oil and gas companies have been particularly interested in the optimal design of pipeline networks together with the size and location of processing facilities to enable maximum hydrocarbon production from wells. The aim of these networks is to gather flows, condition hydrocarbons, and send them to midstream distribution facilities and/or refineries. However, large-scale hydrocarbon production from unconventional wells has transformed the paradigm for facilities planning. First and foremost, the characteristically steep decline of shale wells makes it necessary to continuously develop new wells, whose production needs to be optimally allocated to processing facilities through a more complex network of pipelines. The efficient configuration of a supply chain network can facilitate that task. Recent contributions dealing with the optimal design of the network of facilities servicing shale oil and gas production can be categorized into three groups, according to their scope: processing facilities, pipeline networks and supporting supply chains.

3.6.1 Processing Facilities

Tan and Barton (2016) address the dynamic allocation of mobile plants to monetize shale gas production. Using the Bakken shale play as a case study, they deal with the issue of uncertainty in future supply, demand and price conditions by means of a two-stage stochastic programming approach. They seek to optimally allocate wells to two types of plants: gas-to-liquids (converting methane into heavier hydrocarbons) and liquefaction plants (producing liquefied natural gas or LNG). They introduce 0-1 variables into an MILP model to determine the optimal time to buy, sell and allocate plants of different types to shale sites. The goal is to maximize the expected NPV of the shale gas project. The authors conclude that mobile plants offer a robust way to be profitable even in uncertain conditions.

Allen et al. (2019) also address the sizing and allocation of modular and transportable infrastructure for shale gas processing under uncertain production rates. They introduce the concept of skids that may work in parallel within each processing plant. A superstructure of multidimensional nodes is developed to aid in formulating the problem as a multistage stochastic program. Nodes combine alternative locations, facilities size and technology, and production forecasts. The main decisions are the purchase, allocation and relocation of skids over a multiperiod time horizon. Similar to their previous contribution, the authors conclude that modular units show major benefits over the traditional permanent plants with fixed capacities. More recently, Hong et al. (2020) propose an MILP model to optimally determine the time to purchase and mobilize modular gas processing facilities, as shown in Fig. 13. In contrast to the previous approaches, well pad production start times are also decisions variables in the model, but the problem is solved under deterministic conditions. Curtailing gas production is a feasible option when the processing capacity is not large enough, under the conservative assumption that the production being throttled is directly lost. Similar to the contributions on development planning, this work confirms that the synergistic interaction of production planning with the sizing and dynamic allocation of facilities can increase efficiency.

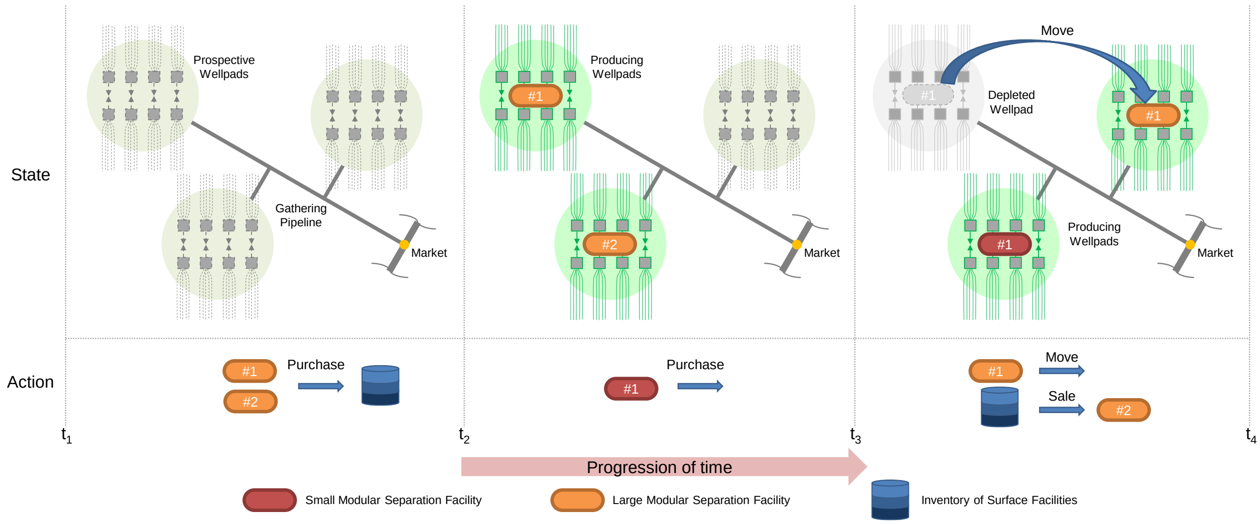


Fig. 13. Simplified illustration of production planning and modular infrastructure dynamic allocation (adapted from Hong, Li, Song, Chen, Zhao & Gong (2020))

3.6.2 Pipeline Networks

Drouven and Grossmann (2017) seek to optimally manage pressure in shale gas pipeline networks together with the planning of turn-in-line operations (i.e., opening of shale wells). Pipeline pressure manipulations permit the reduction of undesirable production backoff and operating costs from gas compression as new wells are brought online, while revenues from gas sales are maximized from an efficient plan of turning new wells into production. The authors propose a multiperiod MINLP model including nonlinear equations to account for pressure drops in gas pipelines and compression power calculations. They also develop a tailored solution strategy to cope with nonconvexities. First, an NLP is used for line pressures initialization; second, an MILP model is solved for pressure bounding; third, a local MINLP solver determines the wells turn-in-line planning; and finally a global MINLP solver seeks to optimize the integrated problem from the incumbent solution. The solution algorithm is used to solve a real-world problem from the Appalachian Basin. In turn, Hong et al. (2020) address the optimal design and planning of pipeline gathering networks over natural gas fields. Hydraulic equations and detailed terrain profiles are accounted for in the selection of pipeline diameters, although nonlinear correlations are approximated by piece-wise linear functions finally yielding an MILP model. An ant-colony algorithm is used to pre-optimize the detailed routes that might be selected by the MILP model to connect the nodes, in a 3D representation. The model also seeks for the optimal location of a centralized processing facility, so that the net present cost of pipeline construction is minimized. The proposed model is applied to three gas fields in China, where well sites are scattered over an undulating terrain with prominent obstacles.

Very recently, Montagna et al. (2022) address the optimal design of pipeline networks gathering multiphase flows from shale oil wells. They develop a comprehensive MINLP formulation to optimally determine the number, size and location of tank batteries and processing facilities together with pipeline diameters and connections, over a multiperiod time horizon. Nonconvex, nonlinear correlations are used to predict pressure drops in multiphase (oil, gas and water) pipelines, which allows the model to properly size pipeline diameters. Due to the problem complexity, the authors develop an NLP-MILP decomposition approach, also implementing refinement strategies to find better solutions. On the other hand, MILP relaxations are devised to tighten bounds on the objective function. A real-world problem from the shale oil industry is solved to a global optimality gap of 5%.

3.6.3 Supporting Supply Chains

Broadening the scope of facility planning problems in the shale oil and gas industry, Tan and Barton (2017) address the optimal design of a country-wide supply chain network, involving multiple shale plays. More specifically, they integrate Bakken, Utica, Marcellus, Niobrara, Permian, Haynesville, Eagle Ford basins in the United States. The aim is to determine the optimal number, location and capacity of three different types of plants (hydro-skimming refineries, gas-to-liquids and LNG plants) to convert shale oil and gas flows into LNG, gasoline, kerosene, diesel and residual fuel oil. Moreover, the model also selects the optimal transportation modes (pipeline, road, rail, barge) to use across the network. To account for uncertainty, different scenarios are proposed, based on future oil prices and Gross Domestic Producttrends. A limiting assumption is that natural gas prices are linked to the oil prices. The authors develop a two-stage stochastic programming formulation whose deterministic equivalent is a large-scale multiperiod MILP. Finally, Montagna & Cafaro (2019) present an MILP model for the strategic design of supply chains providing services and materials (e.g., proppant and steel) to upstream operations, as depicted in Fig. 14. The multiperiod model determines the optimal number, location, capacity, and average response time of facilities from which materials and services are supplied to the field. Like most approaches to facilities planning optimization, the underlying assumption is that the well development plan is given. Interestingly and in contrast to the conventional oil and gas industry, the supply chain design adapts as the drilling activity moves to different shale development areas. To reduce the computational burden, nearby wells with common characteristics are grouped or clustered in a single geographical node, which is usually representative of the way that materials and services are supplied in the shale oil and gas industry.

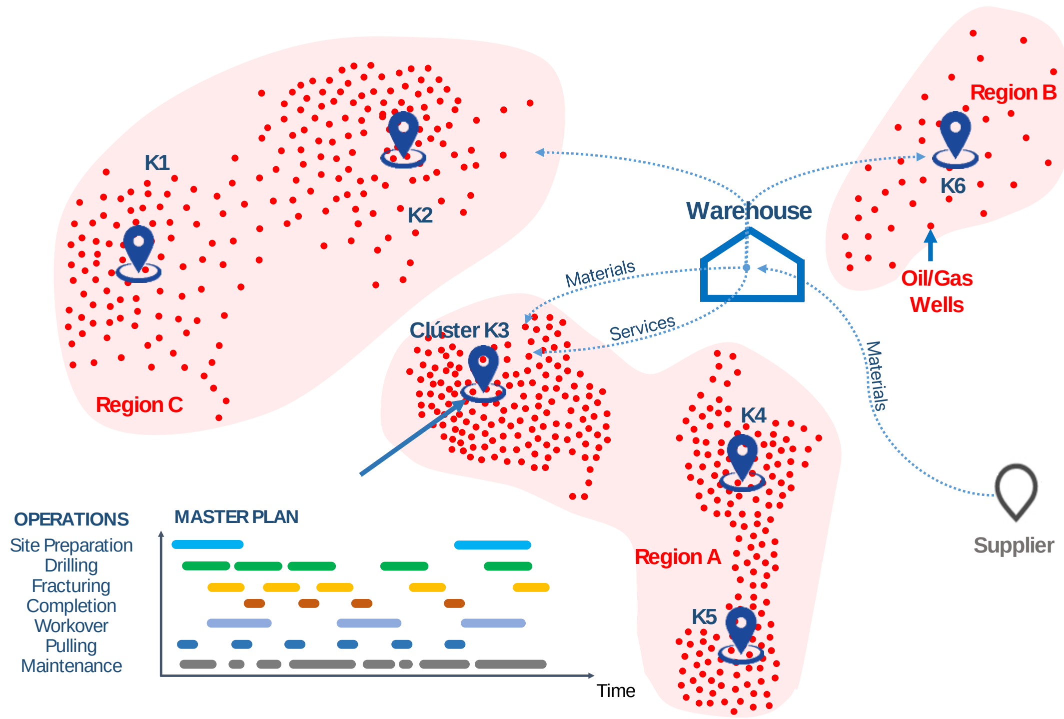


Fig. 14. Illustrative representation of the main elements comprised by the upstream supply chain optimization model and the input data related to every production site (adapted from Montagna and Cafaro, 2019).

3.7 Life Cycle Analysis & Sustainability

Following a comprehensive literature review, particularly focused on optimization tools addressing the environmental impacts of the shale gas industry, Gao and You (2017) identified several key relevant research areas. Based on the need to integrate sustainable design approaches to shale gas energy systems, they provide a series of modeling frameworks that can systematically identify the optimal design and operational strategies while comprehensively accounting for multiple sustainability criteria. In their own words, their series of contributions can be regarded as sustainable optimization at a supply chain (well-to-wire) level. In parallel, life-cycle assessment tools have focused on resource conservation, namely water, air and land, leading to classical Pareto frontiers. As a result, recent contributions in this field can be roughly categorized in these two groups, as explained next.

3.7.1 Resource Conservation

Chen et al. (2017) present a multi-level optimization framework from a life cycle perspective to improve the development of shale gas sites. They develop leader-follower objectives from environmental, economic and energy perspectives, in three subsequent decision levels: the upper level quantitatively assesses life-cycle greenhouse gas (GHG) emissions, the middle level focuses on the benefits for the energy sector, while the lower level seeks to minimize the life-cycle water supply. In a subsequent contribution, Chen et al. (2018) develop a non-rigorous multi-criteria decision making model that integrates life cycle analysis, interval linear programming (to handle inexact data), multi-objective programming, and multi-criteria approaches. The authors argue that, compared with the pure economic optimization scheme, the consideration of environmental objective would lead to roughly 17% reduction of GHG emissions, and freshwater consumption, based on a real application of their framework to the Marcellus shale gas case.

In turn, Wang and Zhan (2019) present an empirical analysis of the sustainable development of the shale gas industry in China. They study the impacts of water shortage, water pollution, pipeline density, geological conditions, market risks and technology, showing that the first three are the major influencing factors for the sustainable development of shale gas in this country. Kroetz et al. (2019) develop an MILP for shale gas gathering pipeline network design accounting for habitat impacts. Based on their results from a real-world case in north Pennsylvania (US), they conclude that the incorporation of impacts associated with both well and pipeline siting encourages more efficient land use in shale gas development. Optimization models to guide the pipeline siting and permitting processes prove to be valuable tools for shale gas companies, communities, and states to identify cost-effective options for land conservation. More recently, in an extension of their contributions to the water management field, Caballero et al. (2020) develop a Life Cycle Impact Assessment (LCIA) of water utilization in shale gas production. The model assesses the most common technologies for water pretreatment and different processes for desalination. Based on economic and environmental results from a bi-criterion MILP formulation, the authors suggest that multiple-effect evaporation with mechanical vapor recompression (MEE-MVR) is the most suitable technology for the wastewater treatment. Besides, they prove that by just ceding 1.06% of the profits, the environmental impact decreases up to 13.5%, as shown by points A and C in Figure 15.

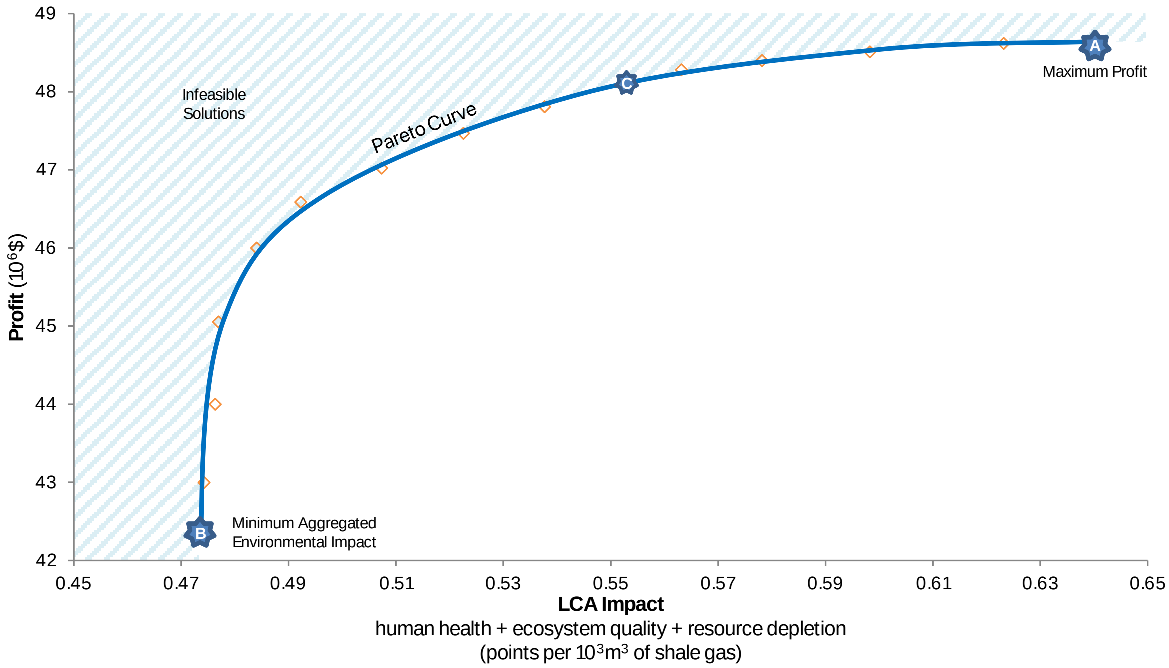


Figure 15. Pareto curve for the minimization of the aggregated LCA environmental impact and maximization of the gross profit (Caballero et al., 2020).

3.7.2 Supply Chain Assessments

Holistic approaches in this field have been proposed in recent years by Gao and You (2017a, 2017b, 2018, 2019). In their seminal contribution, Gao and You (2017a) propose a general modeling framework for the economic and environmental life cycle optimization of supply chains and product systems with noncooperative stakeholders. The framework defines functional-units each of which seeks for life cycle optimization, although a leader–follower Stackelberg game structure is imposed to capture the decentralized decision-making and noncooperative relationships between multiple stakeholders. After solving their MIBLFP (mixed-integer, bilevel, fractional programming) model to global optimality for real instances of the shale gas supply chain, they conclude that the noncooperative perspective provides more insights into the life cycle optimization, and that applications of CCS (carbon capture and sequestration) technologies can lead to significant improvement of the overall environmental performance of the shale gas supply chain.

A second paper of the same research group on the topic (Gao and You, 2017b) presents a mixed-integer nonlinear fractional programming model to investigate the economic and environmental implications of incorporating modular manufacturing into well-to-wire shale gas supply chains. The new model can be viewed as an extension of the previous contribution, leading to the conclusion that design decisions regarding drilling schedule, water management, and midstream infrastructure design and planning are the key factors that led to distinct economic and environmental performances in a shale gas supply chain. In a more recent contribution, the same authors (Gao and You, 2018) address the sustainable design and operations of shale gas supply chains by proposing an integrated hybrid life cycle optimization (LCO) modelling framework that, unlike the traditional process-based LCO that suffers system truncation (from discrete categorizations of LCA), supplements the truncated system with a comprehensive economic input-output system. Finally, to complete their series of works in the subject, Gao and You (2019) develop a dynamic material flow analysis (MFA)-based optimization modelling framework that provides a higher fidelity to model complex material flows with recycling options, also enabling time dependent life cycle material flow profiles. In this case, the problem is formulated as a mixed-integer linear fractional program that is solved by a parametric algorithm. Very recently, Giannikopoulos et al. (2022) address the optimal design of the United States petrochemicals industry using shale hydrocarbons as main feedstocks. The authors develop multi-objective optimization models based on weighted sum and ε–constrained LP formulations that allow elucidating the trade-off between economic costs and net carbon emissions by means of a Pareto frontier. In their network model, the industry is represented as a directed graph, where chemical processes are the nodes and the edges correspond to material and utility flows. Results suggest that moving to low carbon emission points causes a shift towards natural-gas-derived methanol (mainly from shale gas) that is later used for the production of olefins.

Publication	Oil/Gas	Problem Scope	Objective(s)	Degrees of Freedom	Model Type	Solution Strategy	Uncertainty
Gao & You (2017a)	Gas	Upstream, Midstream & Downstream	* Max NPV * Min Life Cycle Impacts of Functional Units	Location and size of facilities; Selection of feedstocks, products and processing technologies, transportation and end use customer supplies.	Leader-follower Stackelberg game - MIBLFP (bilevel, fractional)	Custom global optimization strategy. Parametric, project-based reformulation. Decomp. algorithm.	No
Gao & You (2017b)	Gas	Upstream, Midstream & Downstream	* Min NPC * Min Endpoint Environmental Impact per Electricity Generation	Drilling schedule, well production, water management, sizing of modular LNG plants, routing and sizing of gathering pipelines, electric power generation profiles.	MINLFP (mixed-integer nonlinear fractional program)	Custom global optimization strategy based on a parametric, branch-and-refine algorithm.	No
Gao & You (2018)	Gas	Upstream, Midstream & Downstream	* Min Levelized Cost of Electricity * Min Total LC GHG Emissions per Unit of Electricity	Planning of sites, drilling, well production, water management, location and sizing of processing plants, gathering pipelines and electricity generation.	MINLP	Custom global optimization strategy based on a parametric and a branch-and-refine algorithm	No
Gao & You (2019)	Gas	Upstream, Midstream & Downstream	* Min Levelized Cost of Energy * Min GHG Emission * Min Water Consumption	Planning sites, drilling, pipeline network, processing plants, production profile, water management, transportation planning for water and gas.	MINLP	Parametric algorithm based on Newton's method	No
Caballero et al. (2020)	Gas	Upstream	* Max Gross Profit * Minimize Environmental Impacts	Fracturing schedule, gas production profile, installation of water treatment facilities, flows, storage levels in tanks.	MILP	Commercial solver	No
Wang & Zhan (2019)	Gas	Upstream	None (no optimization)	None. Per region assessment of water shortage, water pollution, pipe density, geological conditions, market risks and technology.	Driving force-pressure-state-impact-response-mgmt. model (DPSIRM)	Empirical: Real-coded accelerated genetic algorithm (RAGA) and projection pursuit (PP)	No
Kroetz et al. (2019)	Gas	Midstream	* Min Costs * Min Habitat Impacts	Pipeline network design. Pipeline development costs and habitat impacts.	MILP	Commercial solver	No
Chen et al. (2017)	Gas	Upstream	* Max Benefits * Min GHG Emissions * Min water use	Number of wells developed, water flows (e.g., freshwater, wastewater transported or reused).	Multi-Level, Linear Programming (MLP)	Clustering of wells and locations.	No
Chen et al. (2018)	Gas	Upstream	* Max Benefits * Min GHG Emissions	Drilling schedule, gas production, water supply/disposal.	MILP	Integration of LCA, multi-objective optim. and multi-criteria analysis.	No

Table 6: Detailed comparison of selected, recent publications on LCA and sustainability in shale operations

4. Critical Assessment & New Research Opportunities for Optimization Models

In the following paragraphs, we critically review recent contributions to the literature in the area of shale oil and gas development optimization. We identify, by major topic areas, opportunities for further research to advance the field in meaningful ways.

In terms of development planning, most work to date has focused on the optimization of regional or even site-specific shale development activities. There have been few contributions dedicated to studying the impact that fully optimized shale development can have on energy supply, climate implications and geopolitical stability at the national or even international level. For instance, the replacement of coal fired power plants with modern natural gas power plants in the U.S. – enabled by the shale gas revolution – has resulted in a significant decrease in CO_2 emissions. In fact, some energy analysts even argue that readily available low-cost natural gas needs to be the centerpiece strategy to fight climate change (Clemente, 2022). At the same time, methane emissions from oil and gas development operations continue to present a major concern (Caulton et al., 2014). Given the existing optimization frameworks, it seems promising for the research community to explore and quantify these tradeoffs so that policymakers and the public can better evaluate benefits and risks in supporting or curtailing shale oil and gas development.

In this context it is also worth noting that, as Tables 2-5 indicate, researchers have embraced the consideration of uncertainty as part of their development planning optimization models over the past few years. Uncertain parameters include water gas price forecasts, production uncertainty and water demand. However, there is a broader uncertainty that challenges the shale oil and gas industry, and that is around political support and the public's perception of the energy sector. As observed by Yergin (2022): "*Many […] believed that demand for oil had peaked in 2019 and would quickly be replaced by renewables. Depressed demand during COVID lockdowns seemed to validate that assessment. An energy transition was thought to be well on its way, facilitated by a wide range of government policies. Yet that perception ran up against reality. Demand for oil and gas bounced back as lockdowns ended and economies rebounded. Furthermore, the war in Ukraine increased the demand of natural gas in Europe given the cuts by Russia in the supply of natural gas. The global energy supply could not keep up, owing in large part to underinvestment in conventional energy sources*." To date, no framework has been proposed to explicitly model and rigorously optimize how uncertainty around hydrocarbon demand at the (inter)national scale could impact (i.e., accelerate or curtail) the development of shale resources by regions or nations. This problem is complicated by the fact that projections for the development of renewables and/or other power sources (e.g., nuclear) must be considered as well. But the opportunity lies in evaluating and quantifying how hydrocarbons produced from shale reservoirs could serve as a means of quickly reinstating energy security to nations dependent on foreign energy. As an illustrative example, Germany – a country strongly committed to ending its reliance on fossil fuels – recently decided to construct multiple large liquified natural gas (LNG) import terminals in response to energy supply disruptions from Russia. The ability to swiftly increase natural gas production and export capacity in response to global disruptions of the energy markets, could pose a significant opportunity for shale producers across the globe.

As can be seen from Figure 7, the field of shale water management has received increasing attention from the optimization community over the years. However, it is remarkable that virtually all work in this area has been focused on produced water from shale gas operations, particularly in the Appalachian Basin. To date, very few researchers have studied how optimization models could support water production associated with oilfields. There are two reasons why shale oil water management is of potential interest: first, the water cut (or: water production associated with oil production) is generally much higher in shale oil basins than in gas-producing development areas. In parts of the Permian Basin, upstream operators produce 9 barrels of water for every barrel of oil. On a basin-to-basin comparison level, the Delaware and Midland basins together produce over 70 times as much water as the Appalachian Basin. Second, investments in water management infrastructure have been far greater in oil-bearing basins. The oil and gas industry has constructed vast and interconnected networks of water pipelines across the states of Texas and New Mexico. These "hydrovascular grids" (Collins, 2021) are facilitating the large-scale recycling of water which is a precious commodity in many arid oilfield regions. Even so, oil and gas organizations in the Permian Basin, for instance, continue to be reliant on the injection of brine into saltwater disposal wells as a means of coping with the massive quantities of water that producers bring to the surface daily. Yet, there has been little work focused on modeling or optimizing produced water injection dynamics and their implications. This is noteworthy since in recent years, produced water disposal has been linked to induced seismicity in Oklahoma, Texas, and New Mexico. In other words, as the industry injected record quantities of water into the subsurface, measurable earthquakes up to magnitude 4.0 and beyond have become a common occurrence. In fact, West Texas has recently been referred to as the "earthquake capital of the U.S." (Bloomberg, 2022). An increase in seismic events – both in terms of frequency and magnitude – could have dire ramifications for the oil industry and energy security in the United States.

Another topic that could be of great interest to the broader shale optimization community is how oil and gas produced water management could contribute to carbon transport and sequestration opportunities. Oilfields across the world already make extensive use of CO_2 for enhanced oil recovery (EOR). CO_2 is oftentimes transported over long distances from carbon capture facilities (e.g., natural gas processing facilities) to EOR well-sites via dedicated high-pressure pipelines. Those very same oil wells continuously bring produced water to the surface. In the U.S. alone, roughly 60 million barrels of water are produced per day – most of which is injected underground for permanent storage. In principle, that water could be carbonated by dissolving CO_2 prior to injection – which would then contribute to carbon sequestration efforts. In fact, the Icelandic company Carbfix (www.carbfix.com) has successfully been co-injecting water and CO_2 for carbon storage purposes since 2014. To the oil and gas industry, co-injection could be of potential interest because it may only require minor changes to existing class II injection permits, and if classified as carbon sequestration, it may qualify for 45Q tax credits in the United States – which are currently set at $50 per ton of CO_2. To put this opportunity into perspective, we refer to a recent article by the oilfield water analytics company, B3 Insight (Wright, 2021), which reasoned as follows: in the Permian Basin alone, roughly 7 billion barrels of produced water are injected every year. At a depth of 800m (which is the typical depth of a class II injection well), about 6kg of CO_2 can be dissolved in every one barrel of water. Therefore, over 40 million metric tons of CO_2 could in principle be co-injected in the Permian Basin alone every year. Considering that the typical passenger vehicle in the United States emits roughly 4.6 tons of CO_2 every year (EIA, 2022), co-injection in the Permian could store the equivalent of 8.7 million vehicles. It is important to recognize that co-injection will not solve the global carbon storage problem, but it could represent a significant contribution towards carbon management efforts. The assessment of these opportunities, and the design of integrated produced water and CO_2 pipeline networks could lead to promising research projects for the shale optimization community.

Finally, in certain parts of the world, oilfield brines are known to have high concentrations of lithium (Kumar et al., 2019). For example, brines produced from the Smackover formation in the United States can contain over 500 mg/L of lithium. This has resulted in solution mining and chemical companies exploring opportunities for lithium resource recovery from produced waters (Lanxess, 2022). Produced water from shale basins across United States has also been shown to contain reasonably high concentrations of lithium (U.S. EPA, 2016). One of the main challenges in this area is that lithium concentrations tend to vary – at times substantially – from one well to the next, even in the same area (Worley, 2019). Downstream mining organizations, however, typically require brine deliveries with relatively consistent feed concentrations for their extraction processes to perform well. One important challenge therefore lies in determining suitable blending strategies for produced waters to pursue lithium recovery at scale. This would suggest that there is an opportunity to develop optimization-based decision-support tools that allow organizations to quantitatively explore opportunities for the recovery of lithium – and potentially other critical minerals and rare earth elements – from produced waters.

In the area of production optimization, recent contributions prove that shale oil and gas production optimization problems are well suited for mathematical programming approaches. Proxy (i.e., algebraic, surrogate) reservoir models are usually embedded into multiperiod frameworks, leading to large-scale, mixed-integer nonlinear programming (MINLP) formulations. Piecewise linear approximations are the most common option to address nonlinearities. On a related note, accurately predicting underground (reservoir) responses to a wide range of interventions is a promising research field that deserves attention from both process systems and reservoir engineers. The effort to keep reservoir models as simple as possible, while being representative enough to capitalize production optimization is still ongoing and has proved to be challenging. Lastly, to date, only two works on shale production planning have addressed the fact that the response of the producing wells to any intervention (even minor, like curtailment) is, in essence, unpredictable. Optimization of carbon capture, utilization, and storage (CCUS) operations is an emerging research topic that may rapidly capitalize knowledge from shale oil and gas production optimization models.

On the topic of Supplies, Gathering and Processing Optimization, transportability, modularity and flexibility to cope with uncertainty and planning dynamics are common features in recent contributions to the optimal allocation of shale wells to processing facilities. If the optimal design of pipeline networks is integrated to the facility planning problem, nonlinear correlations and superstructure-based models need to be simultaneously handled, yielding nonconvex MINLP models with combinatorial complexity (Cafaro et al., 2022). Within this topic, stochastic programming approaches are hardly ever used. Given the problem complexity, optimization approaches for the design of networks for gathering, processing and distributing shale oil/gas and refined products usually rely on the assumption that the development plan is given. The integration of well planning decisions proves to be worth it, but the problem is certainly difficult. Besides that, in practice, drilling programming and facilities planning decisions are usually made one after the other, by different departments within shale oil and gas companies. Moreover, the optimal design of supply chains involving other materials like proppants, massively required by shale oil and gas operations, is still an unexplored area in the literature. Logistics stand for a significant part of the cost, and there is still room for improvement in the supply chains.

Surprisingly, none of the works addressing sustainability in optimization models for shale development deal with uncertainty, in any of its forms. On the one hand, all of these models are based on statistical data that is subject to inaccuracies. On the other hand, energy outlooks foresee many possible scenarios in the way to a totally decarbonized energy matrix. However, no work to date has considered the pace of the energy transition to evaluate their sustainable-optimization models. In fact, only three out of nine works have considered a multi-year time horizon. It is also remarkable that in recent years only shale gas (and no shale oil) projects have been broadly studied and optimized from both economic and environmental perspectives.

Finally, we note that to date, very few shale-centric optimization models appear to have been commercialized into fully supported software decision-support tools. The industry continues to rely on tried and tested database and simulation platforms (e.g., WellView, Aries, Enersight, etc.) that do not make extensive use of mathematical optimization techniques. The main users of the aforementioned software frameworks are drilling, completions, and production, and development planning engineers across upstream, midstream and service companies. This presents an opportunity for the academic community to better understand the typical workflow of its "target audience" in this space, and tailor optimization models to their needs. For instance, considering the capital-intensive nature pipeline buildout projects, it should be very valuable to report an optimality gap on a particular pipeline network design to a development planning engineer. Such a metric can build confidence in utilizing optimization-based decision-making that other approaches (e.g., simulation) cannot offer.

5. Conclusions

This paper has presented a comprehensive review of optimization models for shale oil and gas development. It has first provided a general overview of the operations involved in the production of shale gas and shale oil. Next, it has offered a comprehensive overview of optimization models and solution strategies for addressing development planning, production optimization, supplies, water management, gathering and processing optimization, and life cycle analysis (LCA) and sustainability problems.

In terms of optimization models for development planning summarized in Table 2, it is clear that most of the work has been aimed at shale gas and only very little at shale oil. It is interesting to point out that 4 out of the 11 models take uncertainty into account. Most of the proposed models correspond to MILP problems that are solved by commercial software or tailored decomposition strategies. In terms of shale production optimization models summarized in Table 3, there are NLP, MILP, and MINLP methods, with only 2 out of 8 models taking uncertainty into account. Solution strategies are varied and include reformulation of GDP models, decomposition methods, global optimization, two and multistage stochastic programming.

In terms of water management models summarized in Table 4, there is nearly an equal split between MILP and MINLP models, and only one accounts for uncertainty. Most of the models are solved by commercial solvers. In terms of gathering and processing optimization models summarized in Table 5, there are a few more MILP models than MINLP models, with 3 out of 8 accounting for uncertainty. In terms of life cycle analysis and sustainability models summarized in Table 5, about half are MILPs and the other half are MINLPs. While none of them accounts for uncertainty explicitly, some involve Stackelberg game, multilevel and multi-objective optimization.

From the above, we conclude that mathematical programming techniques, which have been largely developed by researchers in Process Systems Engineering, have played a major role in the optimization of shale and gas development systems. It is also clear that they have showed their value as was for instance documented by EQT Corporation with a produced water scheduling tool that was expected to save the company \$25-35MM per year (EQT Co., 2019).

Finally, we stress that there are a number of outstanding major challenges and issues to be addressed in the area of shale oil and gas optimization, as discussed in section 4. On the one hand there are modeling and computational challenges associated with the capability of handling more accurate nonlinear reservoir models, and expanding the scope of the models for handling larger systems. On the other hand, there is a need to assess the impact of shale gas on the overall energy supply as well as on its impact on the environment. First, long term expansion planning models (e.g., see Lara et al., 2018 and Li et al., 2021) should be incorporated in shale gas models to assess the benefits of incorporating natural gas over time given the increasing penetration of renewables such as solar and wind. Second, it is very important to evaluate quantitatively the potential of decreased CO_2 emissions by replacing coal with natural gas for power generation. Third, there is also a clear need to develop optimal strategies for reusing and recycling of produced water, as well as strategies for reducing methane emissions. Furthermore, there are interesting possibilities for carbon sequestration in shale oil and gas plays, as well as opportunities around lithium recovery from brines. From a modeling point of view, what is needed above all is the integration of LCA and uncertainty in the proposed optimization models (e.g., Azapagic and Clift, 1995) to provide useful tools to both government and industrial decision-makers.

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