# A Model for Shale Gas Wastewater Management

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#### Abstract

Unconventional oil and gas production using hydraulic fracturing generates significant quantities of wastewater that may contain potentially harmful pollutants. The concerns associated with shale gas development necessitate an investigation of shale gas water and wastewater management using a systematic approach to make sure that shale gas development is environmentally sustainable. In this research, we adopt an integrated system analysis approach to examine the life cycle of water in the hydraulic fracturing process. Specifically, we developed a multi-objective programming model for shale gas water and wastewater management that incorporates the objectives of four types of decisionmakers: oil and gas well developers and operators, centralized wastewater treatment facility planners and operators, environmental regulators, and social planners. This paper lays out a modeling framework that can, in the future, be used for a case study of optimal shale gas water and wastewater management. It also provides directions for future expansion of the model.

**Key Words:** Shale gas, wastewater, onsite, offsite, storage, deep well injection, reclaimed wastewater, road damage, earthquake, environmental externality, siting, mathematical programming, optimization

**JEL Classification Numbers:** L95, Q4, Q5

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#### 1. Introduction

Since the mid-2000s, a dramatic increase in the United States' supply of domestic shale oil and gas has been made possible by better subsurface imaging techniques and increased use of horizontal drilling and hydraulic fracturing. These three methods have made extraction of unconventional sources of natural gas, such as shale gas, economically viable and have allowed shale gas to become a significant portion of the American energy supply. The production of shale gas resources is forecast to continue increasing, and by 2040, the US Energy Information Administration (EIA) projects that shale gas and tight oil plays will supply 69 percent of all natural gas produced in the United States (EIA 2016).

Substantial portions of the growth in American shale gas production have come from the Marcellus Shale. The Marcellus is the most expansive shale play in the United States (Kargbo et al. 2010) and is estimated to account for 29 to 55 percent of domestic shale gas reserves (Lutz et al. 2013). The Marcellus Shale underlies 70 percent of Pennsylvania and significant portions of Ohio, West Virginia, and New York as well as small areas of Maryland, Kentucky, Tennessee, and Virginia. The first Marcellus shale gas well began producing in 2005. Gas production doubled between 2010 and 2011 (Hansen et al. 2013), and in 2011 alone, 1,937 wells were drilled in the Marcellus (Maloney and Yoxtheimer 2012). By 2014, the Marcellus accounted for 40 percent of shale gas production in the United States (Kuwayama et al. 2015a).

The rise of fracking and shale gas extraction has been accompanied by controversy over air and water quality, workers' health and safety, economic impacts to local communities, and other issues. Early water-related concerns addressed issues directly related to fracking fluids and additives used in the well stimulation process, such as drinking water contamination from fracking chemicals, but more recently, the focus has turned to the water cycle: water sourcing, water use, wastewater generation, treatment, recycling, reuse, and disposal.

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When fracking a well, millions of gallons of water are mixed with sand and chemicals and injected into the well at high pressure to break up the shale and release oil and gas (Schmidt 2013). Some of this water returns to the surface (referred to as "flowback") along with water originating underground ("produced water"). Wells in the Marcellus produce the majority of wastewater immediately after the fracking operation but will continue to produce water throughout their lifetime. Wastewater (flowback and produced water) usually contains high levels of total dissolved solids (TDS) such as salts and metals, naturally occurring radioactive materials (NORMs), production chemicals (such as friction reducers, biocides, and corrosion inhibitors), residual oil and gas, grease, and other materials (GAO 2012). Marcellus wastewater is known to have high NORM levels (Kargbo et al. 2010). The chemical profile and quantity of wastewater varies with shale play, well location, and well depth, in addition to other factors. This water requires proper treatment to avoid environmental damage or risks to human health, and proper wastewater handling is also necessary to avoid spills and contamination. For a discussion of human health impacts from exposure to wastewater from fracking fluids, see Bamberger and Oswald (2012), Kuwayama et al. (2015b), and Colborn et al. (2011).

In Pennsylvania, four general methods are used to handle wastewater: injection into wastewater disposal wells, partial treatment onsite for reuse and recycling in future fracturing operations, transportation to an offsite centralized wastewater treatment (CWT) facility for reuse (which may include reuse for fracturing or for other beneficial uses), and transportation to a CWT for post treatment surface water discharge. Operators may use multiple treatment options over the lifetime of a well or at one time, based on wastewater quantities and composition and on economic considerations. Other management options, such as evaporation or use in agriculture, are used in other shale plays but are not allowed by law or are not practical in the Marcellus.

Wastewater reuse and recycling<sup>1</sup> are becoming more common because of issues with water sourcing, particularly in drought-stricken areas, or because disposal options are limited by geologic, economic, or regulatory factors. Nationwide, the most common method of managing wastewater is disposal through injection wells, not reuse or recycling (GAO 2012). In the Marcellus Shale, recycling and reuse rates are higher than for other shale plays. This is because there are few disposal wells and a lack of wastewater treatment infrastructure. Pennsylvania has few disposal wells because of

<sup>1</sup> Definitions of "reclaimed," "reused," and "recycled" water vary depending on the information source. In this paper, "reclaimed water" is wastewater that has undergone some level of treatment, "reused water" is wastewater that is reconditioned or reclaimed for subsequent hydraulic fracturing or used for a nonfracking beneficial use, and "recycled water" is wastewater that is treated for discharge to the environment.

unfavorable geology (Abdalla et al. 2011). Thus, well operators either dispose of wastewater in wells in Ohio or West Virginia, which requires them to pay high transportation costs, or they treat wastewater at treatment plants or onsite.

Wastewater reuse can provide several benefits. It reduces freshwater withdrawals, which saves transportation and pumping costs, reduces truck traffic or use of (or even need for) pipelines to carry water, and reduces the need for water storage in pits. These reductions in turn reduce spill risks, truck accidents, and road damage. In addition, recycling and reuse are economically appealing for operators when disposal costs are high, or if wastewater will only require minimal treatment before reuse in fracking operations or for other beneficial uses. However, wastewater recycling and reuse may not eliminate the need for wastewater disposal, and the liquid waste remnants of water treatment processes will have higher concentrations of heavy metals and other chemicals, raising the consequences of a spill should one occur during transportation or elsewhere in the disposal process. Also, recycling and reusing wastewater may not be the cheapest option for all wells or for all periods. The costs of onsite storage capacity to store wastewater and the costs of onsite treatment options, including the costs of energy to run the equipment or transportation to treatment facilities, can make treatment and reuse prohibitively expensive (Cooley et al. 2012).

Wastewater reuse for fracturing is only a temporary solution because maturing well fields become net water producers over time (Vidic et al. 2013). Reuse of all produced water is possible only while the number of new wells being constructed surpasses the number of wells in production (Lutz et al. 2013). This problem is viewed as a reason to develop additional treatment methods and ways to recycle wastewater. Managing wastewater is a growing challenge: the volume of unconventional oil and gas wastewater requiring treatment and disposal has continued to grow despite a slowing in drilling and production (Figure 1; see Appendix for further details).

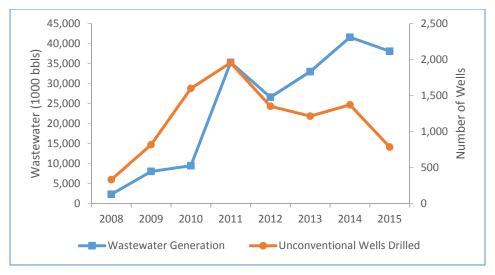


Figure 1. Wells Drilled and Wastewater Generation in Pennsylvania, 2008–2015

Source: Wastewater: PADEP (2016c); Wells Drilled: PADEP (2016b)

Operators need to evaluate the economics of recycling and reuse, considering the cost of water acquisition, transport, and disposal relative to the cost of any storage, treatment and transportation that must occur for wastewater recycling and reuse. High disposal costs have led to increased reuse of wastewater, replacement of fresh water with brackish water, reduced disposal volumes, and more local and onsite water treatment; in addition, more large wastewater management suppliers support multiple components of the water management process, and transportation methods have changed, with a higher reliance on pipes and onsite treatment to minimize trucking costs (Gay and Slaughter 2014). Besides private costs to producers, shale gas development poses potential social costs, such as surface water and groundwater pollution, methane leakage, conventional air pollution, traffic accidents, accidental spills, and road damage.

Managing wastewater from shale gas production is a significant factor that will affect both the economics of shale gas development and human and environmental health (Shaffer et al. 2013). It is therefore imperative to model and understand the life cycle of water and wastewater management, considering the economic and environmental factors associated with system inputs and outputs. Such modeling could illuminate optimal wastewater management strategies as well as the trade-offs involved with each management decision.

Thus, the goal of this research is to develop a modeling framework to facilitate understanding of the life cycle of water and wastewater generation processes of shale gas production and the trade-offs associated with various management options. The ultimate goal is to provide tools to both

operators and government regulators to improve the economics and sustainability of shale gas development.

Specifically, we develop a multi-objective dynamic optimization model for shale gas water, wastewater, and solid waste management and resource recovery. The model is developed with four decisionmakers in mind: oil and gas well developers and operators, centralized wastewater treatment facility planners and operators, environmental regulators, and what economists call social planners people and institutions, such as community groups and governments, interested in the welfare of all of society. In addition, the model can describe outcomes and trade-offs when operators also own waste treatment facilities or otherwise take into account waste treatment facilities' behavior. For well developers and operators, the objective is to minimize costs from water and wastewater management and disposal. For centralized wastewater treatment planners and operators, the objective is to minimize the cost of capital and operations and maintenance (O&M) to build and operate a wastewater treatment facility and maximize the revenue from selling reclaimed water and other recovered resources. For environmental regulators, the objective is to minimize environmental damage (such as pollutant loading in surface water discharge), ensure compliance with effluent standards, and minimize population exposure risks. For social planners, the objective is to minimize social costs, which encompass private costs plus environmental costs (also called externalities). Although the modeling framework could potentially be generalized to other unconventional fossil fuels, at this stage we focus on shale gas development.

The rest of the report proceeds as follows. Section 2 characterizes the water and wastewater life cycle during shale gas development. Section 3 reviews the mathematical models of water management in the shale gas industry currently in the literature and presents our model's additions to that literature. Section 4 describes the model development. Section 5 discusses model solution and data issues. Finally, Section 6 provides a conclusion and discussion of future work.

# 2. Characterization of the Water and Wastewater Cycle

The hydraulic fracturing water and wastewater life cycle consists of water acquisition and consumption, wastewater generation, freshwater and wastewater storage, transportation of fresh water and wastewater, wastewater treatment, onsite reuse, reclaimed water use (including beneficial reuse), wastewater disposal, and surface water discharge. We discuss these processes in the sections below. We also discuss wastewater management options, solid waste generation, and environmental impacts.

# 2.1 Water Acquisition and Consumption

Large volumes of water are needed to drill and fracture shale gas wells. Requirements differ by location within and between shale plays because of geologic conditions, but in general, extracting shale gas from horizontal wells by hydraulic fracturing requires more water than is needed for conventional wells: the wells must be deeper to access shale deposits, horizontal drilling creates longer wellbores, and most importantly, water is needed for the fracturing process itself (Vidic et al. 2013). In terms of water intensity—the volume of fresh water consumed per unit of energy in the fuel produced—shale gas is more water intensive than conventional gas but less water intensive than conventional oil, on average (Kuwayama et al. 2015a).

About 80,000 gallons of water is needed to drill a shale gas well in the Marcellus (Veil 2010), but much more water is needed to fracture the well. Jackson et al. (2015) estimate that the average well in Pennsylvania during 2008 through 2013 used 4,460,000 gallons of water. Chesapeake Energy reported using 85,000 gallons for drilling and 5,500,000 gallons for fracturing an average well in the Marcellus (Mantell 2011).

During the fracking process, water (though other base fluids can be used) is mixed with proppants (such as sand) and chemical additives, then pumped into the well under high pressure to create fissures in the shale to release trapped oil and gas (Elsner and Hoelzer 2016). The composition of fracturing fluid differs between wells as well as for different periods of the fracturing process. The mix of chemicals that are included in the fracturing fluid is determined by the chemical conditions of the water and shale and the functions that the fracturing fluid is needed to perform (Elsner and Hoelzer 2016). In the Marcellus, chemical additives commonly include friction reducers, scale inhibitors, and biocides. Base water used for fracking fluid does not need to be drinking water quality; produced water with high TDS concentrations has been used for some well stimulations (Lebas et al. 2013). Brackish water, treated industrial water, treated municipal wastewater, and recycled water from other fracking operations can all be used for well stimulation, depending on the chemical composition of the water and the composition of the shale formation.

Most fresh water used for Marcellus wells comes from surface water (Freyman 2014), with only 20 percent coming from groundwater sources (EPA 2015b). In Pennsylvania, the dominant source of water used by operators is water withdrawn from rivers and streams (EPA 2015b). Despite the large quantity of water required to drill and fracture each well, water use for fracturing shale gas wells in Pennsylvania accounts for less than 1 percent of all available surface water in the state (Hansen et al. 2013). Nationwide, fracking accounts for less than 1 percent of total annual water use, though fracking in some counties uses a much larger percentage (EPA 2015a). Even in areas with

seemingly low overall water use, local effects can be large, especially during times of drought or when large quantities of water are removed in a short time. In the Marcellus Shale, small rivers, creeks, and streams with drainage areas of less than 100 square miles, which are more vulnerable to damage from large, sudden withdrawals, supply 40 percent of surface water used for fracking (EPA 2015b; Kuwayama et al. 2015a). Even though the Marcellus is not as vulnerable to drought as other shale formations, in 2010, 2011, and 2012, the Susquehanna River Basin Commission (SRBC) suspended withdrawal permits for some streams exhibiting low stream levels (Detrow 2012). The Marcellus Shale underlies three major river basins in Pennsylvania: the Susquehanna River basin, the Delaware River basin, and the Ohio River basin. For water from the Susquehanna River basin, which spans Pennsylvania, New York, and Maryland, operators must first obtain permits from the SRBC. Roughly 13 percent of the injected fluid in the Susquehanna River basin is reused wastewater; all other water is from freshwater sources (EPA 2015b). The SRBC requires a permit for all water withdrawn from surface water or groundwater sources and all water used consumptively for unconventional oil and gas development, regardless of the amount. 2016 regulations for the SRBC outline three possible fees that natural gas well operators could face: a project review fee of \$10,000, a project review modification fee of \$1,125, and a consumptive use mitigation fee of \$0.33 per 1,000 gallons of water consumed<sup>2</sup> (SRBC 2016). Withdrawals from the Ohio River basin are not controlled by a central agency, so withdrawals in Pennsylvania areas of the basin are regulated by the Pennsylvania Department of Environmental Protection (PADEP) (ORSANCO 2015). PADEP has a registration program for withdrawals exceeding 10,000 gallons per day and requires annual reporting from all registered water users. The Delaware River Basin Commission (DRBC) has imposed a moratorium on drilling activity since 2009, so no water is currently being removed from that basin (Phillips 2016).

Removing large quantities from surface water sources can affect hydrology, hydrodynamics, and ecosystem health; groundwater removals can cause land subsidence, mobilize naturally occurring elements and contaminants, and promote bacterial growth (Cooley et al. 2012). Such effects on water quality and quantity can conflict with other needs, such as agriculture, recreation, and ecosystem health.

<sup>&</sup>lt;sup>2</sup> This fee is just one of several mitigation options that project sponsors can choose. All water used for shale gas development is considered to be consumptively used; well operators pay the mitigation fee for all consumptively used water, with the exception of flowback or produced water reused for fracking.

#### 2.2 Wastewater Generation

During the hydraulic fracturing process, water, chemicals, and proppants are injected under high pressure. When the pressure is released, water that was forced into the well returns to the surface and the well begins to produce wastewater. Hydraulic fracturing produces two types of wastewater: flowback and produced water. Flowback is hydraulic fracturing fluid injected into the well that returns to the surface. Reported flowback levels for the Marcellus Shale range between 10 and 40 percent of the initial volume of fracturing fluid but are often less than 20 percent (Gregory and Mohan 2015). Produced water is the naturally occurring underground water that is brought to the surface as part of the fracturing and production process. Flowback usually comes to the surface during the first three to four weeks following well stimulation, preceding oil and gas production. The highest rate of flowback occurs on the first day and then declines over time (Gregory et al. 2011). One source reports that 60 percent of flowback emerges in the first four days after fracturing (URS 2011). Flowback accounts for around a third of all wastewater generated from fracking a well (Lutz et al. 2013). In the Marcellus, a normal well may produce 1,200 to 1,500 barrels of flowback for a few weeks after fracking the well and then the rate will decline to only a few barrels a day of produced water for the remainder of the well's life, which may be as long as 20 years (Gay and Slaughter 2014). Produced water has a higher concentration of TDS than flowback (Gregory and Mohan 2015), and the concentration of dissolved salts increases dramatically over time (Haluszczak et al. 2013). Some wastewater reports do not distinguish between flowback and produced water because they consider flowback a component of produced water, and others contend that it is not possible to differentiate between the two types of wastewater (Cooley et al. 2012).

Wastewater management must account for introduced chemicals added to fracturing fluids and chemicals naturally found in geologic formations, which are more heavily concentrated in produced waters. Shih et al. (2015) analyzed wastewater sample data from PADEP and found that median concentrations of several substances, including TDS and NORMs, were significantly higher in produced water than in flowback. The Marcellus Shale is considered to have higher levels of NORMs, TDS, metals, and organic matter than other shale plays, a difference that increases the complexity of wastewater management (Steinzor and Baizel 2015). High concentrations of NORMs and other chemical constituents that exceed safe drinking water limits require careful handling to avoid spills and proper treatment before reuse, discharge, or disposal to avoid contaminating surface water and groundwater. Reuse, treatment, and disposal can occur either onsite or offsite, as discussed below. Management decisions are constrained by available technology, regulations, geology, chemistry, and ultimately the cost of disposal and treatment options. Operators want to minimize treatment and

disposal costs because storing, treating, transporting, and disposing of produced fluid can be one-third to one-half of a producing well's total operating expenses (IHS 2013).

Both conventional natural gas production and unconventional shale gas production generate produced water. Hydrofracked wells generate more wastewater overall but are more efficient because they generate 35 percent less wastewater per unit of recovered gas (Lutz et al. 2013). Despite increased efficiency, given the large number of existing wells and the predicted growth in shale gas extraction, the total amount of wastewater from shale gas wells will continue to grow. There is a linear correlation between natural gas production and the volume of produced water generated from shale gas extraction (Karapataki 2012): if shale gas production reaches the projected levels cited above, wastewater management will become an even greater problem than it currently is. Already, the growth in fracking has generated a six fold increase in wastewater between 2004 and 2011 (Schmidt 2013).

# 2.3 Storage

Designing and sizing water storage systems is a critical component of any water management plan. Water can be stored in pits or frack tanks, and different types of pits and tanks are used to store wastes during different stages of oil and gas development (Kuwayama et al. 2015b).

Water brought to a well site must be stored before use in drilling or hydraulically fracturing a well.<sup>3</sup> The primary type of frack tank holds 21,000 gallons and can be transported by a tractor-trailer (URS 2011), but the size and number of tanks needed, as well as the cost to lease or acquire them, vary (Hefley et al. 2011). Once wastewater comes to the surface, it is usually stored in pits or above-ground storage tanks before treatment. Pennsylvania regulations differentiate among temporary pits used during drilling and fracturing, pits used to hold produced water, and centralized impoundments used to hold wastewater from several well sites (Kuwayama et al. 2015b). Pits can hold hundreds of thousands of barrels of wastewater, but tanks, despite their smaller capacities, may be more appealing to operators because they offer more flexibility and pose fewer environmental risks (Gay and Slaughter 2014). Impoundments are used for the same purposes as production pits but are much larger (some store tens of millions of gallons of fluid) and may serve a wide geographic area (Steinzor and Baizel 2015).

Several environmental risks are associated with water storage systems. These include groundwater contamination from leaking or overflowing pits; surface spills; the release of odors and

<sup>3</sup> Centralized freshwater impoundments are also an option, where water is stored prior to moving to the wellsite.

air contaminants, such as volatile organic compounds; and harm to livestock and wildlife, such as deer and birds, that come in contact with impounded water (Ramirez 2009; Adams et al. 2011; Kuwayama et al. 2015b; Steinzor and Baizel 2015). Contamination from wastewater storage can occur through volatilization and vaporization of contaminants, surface spills and runoff, and leaching into groundwater, but the most common causes of wastewater release are pit overflows, tank overfills, and liner malfunctions (Kuwayama et al. 2015b). Because of the risks from wastewater storage, Pennsylvania, like many states, regulates water storage infrastructure and requires regular inspections. In 2010, 25 percent of environmental violations in Pennsylvania were associated with pit and storage problems, such as leaks, and between 2006 and 2012, 30 percent of fracturing fluid and chemical spills were from fluid storage units (EPA 2015a). The primary violations for improper management are structural instability, improper encapsulation, liner holes, liner tears, fluid leaks, seepage of contaminated fluids, and erosion and runoff from pits (Steinzor and Baizel 2015). Based on data from Colorado, New Mexico, and Oklahoma, Kuwayama et al. (2015b) report that tanks are associated with fewer and smaller spills than pits, but the fluids that they spill tend to present greater risks to environmental health; moreover, tanks generally face fewer regulations than pits.

Storing flowback in enclosed tanks has been recognized as a best management practice for many but not all sites because it reduces emissions, runoff, and contact with wildlife (Lewis 2012). In addition, tanks can be more closely monitored for leaks and are more suitable than pits for regions with heavy precipitation events, which may cause pit overflow, and for areas with shallow groundwater tables (Kuwayama et al. 2015b). However, tanks are less commonly used because of higher costs (Gregory and Mohan 2015), and they can pose higher risks in some locations. The cost of building a storage pit depends on its size and the site conditions (such as topography and terrain), but on average, the costs are about \$120,000 to build a pit and \$60,000 to \$70,000 for lining it. Fencing and maintenance costs usually are minor (Hefley et al. 2011). Produced water is collected in enclosed tanks, where it is separated from oil and gas (Gregory and Mohan 2015). Usually, operators employ a combination of impoundments, pits, and frack tanks to manage wastewater (URS 2011). Many tanks are needed to hold all the fracturing fluid or flowback, especially during periods of high flowback production, but this management system offers more flexibility than onsite impoundments.

States have the sole regulatory authority for the storage of shale gas wastewater in impoundments because oil and gas wastes are exempt from the Federal Resource Conservation and Recovery Act (Hammer et al. 2012). Pennsylvania governs the transportation, storage, and disposal of wastewater under its Solid Waste Management Act (Hammer et al. 2012). Pennsylvania law prohibits water pollution from impoundment sites and enforces this policy by requiring operators to obtain permits and create water quality management plans and by providing construction and design

guidelines (Hammer et al. 2012). In February 2012, Pennsylvania restricted the ability of local governments to regulate siting and zoning of new impoundments (Hammer et al. 2012). Pennsylvania has limited the construction of impoundments and holding tanks in floodplains and has added inspection requirements to limit contamination from impoundment overflow and stormwater runoff. In addition, the state requires synthetic liners for all containment ponds. On January 6, 2016, PADEP released the final rulemaking package for amendments to 25 Pennsylvania Code Chapter 78a, concerning surface activities associated with unconventional oil and gas well development. The amendments differentiate establish construction standards for impoundments, ban the use of pits or larger centralized impoundments to store drill cuttings and waste fluids (with exceptions for small pits that obtain a permit) for unconventional operators, require monthly maintenance inspections for tanks, require secondary containment for all storage vessels, and require operators to create a water management plan (DEP 2016). The amendments were approved by the Pennsylvania Environmental Quality Board on February 3, 2016 (EQB 2016).

Storage and impoundment play critical roles in shale gas water and wastewater management. They provide not only temporary storage of flowback, produced water, and other fluids at oil and gas production sites, but also a buffer to reduce the peak flow rate and concentration load for wastewater treatment; hence they reduce wastewater treatment costs. However, these storage facilities for contaminated wastewater may release harmful substances and ultimately lead to human and ecological exposures. See Kuwayama et al. (2015a) for a detailed discussion of the human and ecological risks associated with various storage facilities and the costs and benefits of various options for mitigating risks from onsite storage of wastewater.

# 2.4 Water and Wastewater Shipment

Water acquisition for hydraulic fracturing and disposal of flowback and produced wastewater requires shipping large quantities of water. Unless all these needs can be met by onsite sources or very nearby sources of surface water, groundwater, or reused wastewater, water must be brought to the well pad by pipeline or truck. Similarly, wastewater and other waste products from fracking must be removed from the site via pipe or truck, except for the waste materials that will be reused or disposed of onsite. Transportation costs can be high and strongly influence wastewater management choices. Onsite recycling and reuse decrease the amount of water that must be brought to the site as well as the amount of contaminated wastewater to be removed for treatment and disposal.

The two transportation methods are discussed below.

#### **2.4.1 Pipes**

Transporting water via pipe (also referred to as "water transfer") is often more economical than transportation by truck if the travel distance is under five miles (Gay and Slaughter 2014). Operators need to choose between permanent underground pipes or above-ground pipes. EQT Corporation reported paying \$90 per foot of pipeline to rent pipe to pump water to its site (Hefley et al. 2011). In 2013, Antero Resources announced plans to build an 80-mile pipeline to carry water from the Ohio River to fracking sites in West Virginia and Ohio. Despite the huge projected cost—half a billion dollars—the company predicted savings of \$600,000 per well and said the pipeline would cut the company's water costs by two-thirds (Gold 2013). Pipelines do have downsides—they are linked with leaks, spills, and right-of-way controversies (Cooley et al. 2012)—but leaks or spills of fresh water do not pose pollution risks.

#### **2.4.2 Trucks**

Water hauling via truck is usually done with 130-barrel tank trucks and is usually more expensive than transportation by pipe; however, it offers larger range and operational flexibility (Gay and Slaughter 2014). Each Marcellus well can require 625 to 1,148 heavy truck trips for equipment, materials, and waste (Korfmacher et al. 2015). Transporting water by truck can cost between \$85 and \$175 per hour per truck (Karapataki 2012), and it has been estimated that treating flowback for reuse onsite instead of transporting the flowback can save more than \$150,000 per well, which can mean a 38 percent reduction in transportation costs (Gay and Slaughter 2014). These cost savings from reducing wastewater and freshwater transportation give operators in the Marcellus play significant incentive to reuse as much wastewater as possible. In addition, operators in the Marcellus are often held responsible for road damage caused by heavy truck traffic and have the responsibility to maintain roads; reducing truck trips will reduce this expense (Yang et al. 2014).

The downsides of increased truck transport from drilling and operating oil and gas wells have been a focus of concern for local communities and other stakeholders and researchers. Trucks cause noise and air pollution, increase traffic near well sites, cause wear and erosion on local roads, increase traffic accidents, and increase risk of spills; new roads built to reach rural locations can cause habitat fragmentation and other ecological disturbances (Cooley et al. 2012). Figure 2 compares the rates of accidents involving tank trucks in Pennsylvania counties having 20 or more wells with those of counties having fewer than 20 wells. This empirical analysis found that one additional well drilled per month raised the frequency of accidents involving a heavy truck by more than 2 percent. On average, nine such crashes occur per county per month. Further, Graham et al. (2015) studied motor vehicle accidents in Pennsylvania and found that heavily drilled counties had higher rates of vehicle crashes

and heavy truck crashes than regions without drilling, and that crash rates increased during periods with more drilling activity in counties with heavy drilling.

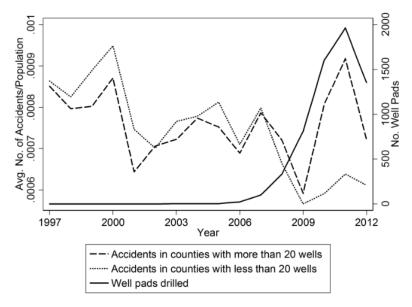


Figure 2. Traffic Accidents and Shale Gas Development, 1997–2012

Source: Muehlenbachs and Krupnick (2013)

Korfmacher et al. (2015) estimated that onsite recycling can reduce the total number of truck trips by 20 percent, lowering costs for operators and also decreasing emissions and other environmental, health, and economic harms of truck transportation. In addition to the risks posed by spills during trucking, transport by truck can also lead to other environmental damage from emissions of carbon dioxide, nitrogen oxides (NO<sub>x</sub>), sulfur dioxide (SO<sub>2</sub>), and particulate matter and can increase congestion and accidents. In turn, accidents involving waste transport trucks can cause wastewater spills. The magnitude of this damage depends on local factors.

#### 2.5 Wastewater Pathways

Several options are available for managing flowback and produced water. Practices differ between operators and between shale plays and have changed over time with regulatory and technological developments. Nationwide, on average, about 90 percent of produced water is disposed of via injection wells (GAO 2012); only 5 percent of injected water is reused wastewater (EPA 2015a), with almost no reuse in some shale plays (Gregory and Mohan 2015). Disposal using injection wells is limited in Pennsylvania and is therefore much more expensive and much less common for Pennsylvania operators. Maloney and Yoxtheimer (2012) report that in 2011 in the Marcellus, 90 percent of flowback water and 55 percent of produced water were recycled, such that 18 percent of

water injected as part of the fracturing process was recycled water (Maloney and Yoxtheimer 2012). Flowback is more amenable for recycling and reuse than produced water because of its lower salinity (Maloney and Yoxtheimer 2012). For flowback to be viable for reuse, oil, grease, hydrocarbons, suspended solids, and iron have to be removed. Feasible reuse options depend on wastewater composition, the treatment capabilities of available technologies, and storage capacity (Karapataki 2012). Operators use multiple management options during different periods of the well's lifespan and for different types of waste. Research and development by industry and universities continues to expand the number of treatment options and performance of onsite and offsite treatment options. As a result, feasible treatment options and their respective performance and costs continue to change and evolve. Regulatory changes at the state or national level have also influenced wastewater management. On July 13, 2016, EPA finalized a rule<sup>4</sup> that contains a zero discharge pretreatment standard establishing a zero discharge pretreatment standard for discharges of wastewater from onshore unconventional oil and gas extraction from publicly owned treatment works (POTWs) (EPA 2016). The rule does not address wastewater from conventional oil and gas or injection disposal.

Figure 3 presents wastewater management practices by year, according to data from PADEP waste reports for fracking fluid waste, produced fluid, and brine.<sup>5</sup> Waste management options are normalized by year to show the percentage of wastewater in each management pathway. This figure illustrates the low injection disposal rates in the Marcellus, especially compared with the national average of 90 percent and the relatively high levels of reuse and recycling. It also shows shifts that have occurred over time due to regulatory changes and technological and economic developments that have made various management options more or less feasible. Specifically, the data show the effect of the regulatory changes in 2010 and 2011, such as the more stringent effluent standards for surface water discharge and the ban on shipments of wastewater to POTWs. Additionally, during the period with highest well drilling activity in 2010 through 2012, injection disposal wells and CWT facility recycling both began to receive larger shares of wastewater.

<sup>&</sup>lt;sup>4</sup> Effluent Limitations Guidelines and Standards for the Oil and Gas Extraction Point Source Category. Docket ID EPA-HQ-OW-2014-0598.

<sup>&</sup>lt;sup>5</sup> See Appendix for description of data and methods used to create Figure 2.

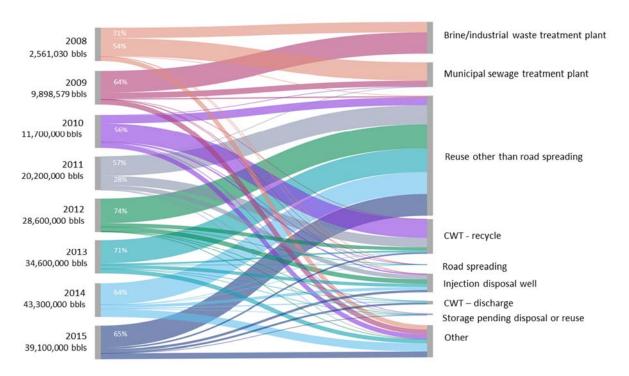


Figure 3. Wastewater Generation and Management Options in Pennsylvania

Note: Reuse other than road spreading includes recycling water for use in fracking.

Source: PADEP (2016c)

The most common treatment methods currently in use are described below; Section 4.3 discusses management options that are included in our model.

#### 2.5.1 Treatment Technologies

Concerns about water availability and wastewater disposal have increased interest in water recycling and reuse in many shale plays and have spurred research and development of water treatment technologies. Complete wastewater reuse for fracking will decrease freshwater volumes needed for subsequent Marcellus Shale wells by 10 to 30 percent (Mantell 2011) and can save operators money, depending on the cost of fresh water and treatment processes. However, operators that reuse all of their flowback and produced water will still need to acquire more water (either fresh or treated) because only a fraction of the water inserted into a well returns to the surface, and fresh water is still the dominant source of water used in well stimulation in most shale plays (EPA 2015b).

Treating shale gas flowback and produced water usually involves a series of treatment steps, depending on the chemical profile of the wastewater and the purpose for the treated water. Each treatment stage and technology target certain specific chemical constituents that can determine the effectiveness of reused wastewater. Constituents of concern in produced water include dissolved and

suspended organics, such as oil and grease; suspended solids, such as formation solids, corrosion and scale products, and bacteria; additives such as proppants, friction reducers, biocides, and corrosion inhibitors; naturally occurring radioactive material, specifically barium and radium isotopes; and TDS, including salts and heavy metals. Reducing the TDS concentration is the primary consideration when treating produced water so that it reaches a quality suitable for discharge or reuse. For a discussion of the contaminants of concern for reuse, see Karapataki (2012). There is no standard water quality that operators need to achieve before reusing wastewater in fracking operations. Rather, requirements depend on the chemical composition of the shale formation and the willingness of operators to risk damaging equipment (because of scaling and corrosion) or otherwise reduce well production.

In general, wastewater treatment options can be classified into four treatment levels: primary, secondary, tertiary for fracking reuse, and tertiary for surface discharge or beneficial reuse (Gao and You 2015; Karapataki 2012). Primary treatment involves clarification only, in which suspended solids, free oil and grease, iron, and microbiological contaminants are removed. The common technologies for primary treatment include coagulation, flocculation, filtration, and disinfection. Secondary treatment involves softening and clarification and removal of ions, such as barium, calcium, magnesium, and strontium, often using lime, to prevent scale formation during the hydraulic fracturing process. Tertiary treatment for fracking reuse is wastewater pretreatment using clarification and softening to remove chloride and TDS, followed by partial desalination. Water is treated to reach a specified contaminant level and then blended with makeup (fresh) water for fracking reuse. The highest level of treatment is tertiary treatment for surface discharge or beneficial use. Under current PADEP effluent standards, wastewater must be treated until TDS is below 500 ppm. The water quality level of treatment for other uses varies. Tertiary treatment may involve partial or complete desalination, with four main technologies: membrane-based technologies, such as reverse osmosis, forward, osmosis and membrane distillation; electrically driven membrane separation, such as capacitive deionization and electrodialysis reversal technologies; thermal technologies, such as distillation, multistage flash, and vapor compression; and zero-liquid discharge technologies, such as crystallization, evaporation, and concentration (Karapataki 2012). Some desalination technologies have specific influent concentration requirements. For example, reverse osmosis may require influent TDS concentration to be lower than 40,000 ppm; to avoid damaging equipment and to maximize the effectiveness of the treatment process, saltier wastewater needs blending or settling before undergoing treatment (Karapataki 2012).

#### 2.5.2 Onsite Treatment

Wastewater can be reused onsite, with or without treatment, to frack additional wells on the same well pad or to conduct additional frack jobs on the same well, without transportation to an offsite water treatment facility. Operators that treat wastewater before blending and reusing it need to decide what level of cleanliness they want. TDS, sand, and other chemicals in flowback and produced water can plug wells, decreasing production, or damage equipment because of scaling and corrosion (Mantell 2011). Onsite direct reuse without treatment incurs minimal cost but presents the highest possibility of well plugging, scaling, and corrosion (Abdalla et al. 2011). Onsite treatment reconditions the wastewater, but reuse still presents moderate potential for well plugging, equipment damage, and reduced well performance (Karapataki 2012). Regardless of the amount of processing that wastewater has undergone, it must be blended with fresh makeup water to satisfy the specifications for reuse in hydraulic fracturing.

The onsite treatment process may include primary, secondary, or tertiary treatment before the fluid is reused. Onsite treatment is usually performed by commercial water treatment companies using a mobile treatment unit (MTU). Wastewater is processed in MTUs and then blended with fresh water to meet the reuse specification for hydraulic fracturing. MTU can be a cost-effective approach—no transportation cost is involved—but onsite treatment is limited by capacity and technical constraints. Treatment volumes are generally limited and the technology can be expensive. The variability among locations, operators, shale chemistry, wastewater chemistry, and fracking fluid additives presents two challenges for the onsite treatment development process: it limits the utilization potential of certain technologies and can make it difficult to produce fracking fluid with the correct chemical composition (Karapataki 2012).

In the Marcellus region, shale gas producers currently manage most produced water through internal direct reuse without desalination to remove dissolved solids. This reuse strategy works under currently low energy prices but is only a temporary solution. As shale gas production in the Marcellus Shale play matures and/or energy price rises, opportunities to reuse produced water in developing new wells will decline while generation of produced water from established wells will continue and the supply of produced water will grow. When produced water volumes exceed demand for internal reuse, producers in the region will be driven to explore other options for reuse (Shaffer et al. 2013) or will increase discharge amounts.

#### 2.5.3 Offsite Treatment

As the number of wells and volume of wastewater increase, using MTUs to treat the flowback and produced wastewater at the wellhead may become cost prohibitive or infeasible for reasons such

as inadequate water storage capacity or inability to quickly reuse the water. In such cases, a semipermanent, centralized system is necessary. Unlike MTUs, centralized wastewater treatment plants can provide a broader scope of treatment options and have a larger capacity. CWTs have lower treatment costs per gallon due to economies of scale and can also consider other recovery of resources such as gypsum and salts. Moreover, unlike typical MTUs, CWT facilities can take water from all stages of a well's lifespan and take water from multiple wells.

Some CWT facilities treat water for discharge; others treat water for reuse; others do both (Karapataki 2012). Water treated for discharge must meet PADEP effluent quality regulations, but wastewater treated for reuse can vary in the quality of treatment.

Major disadvantages of centralized systems are high capital costs, reduced flexibility, and potentially high transportation costs. Centralized systems built in a modular fashion will be more flexible: capacity can be brought online in stages as produced water flows and volumes rise. Transportation costs can be lowered through siting optimization and, depending on a well's location, by transporting wastewater via pipe.

# 2.6 Deep Well Injection

Nationwide, the most common management option is disposal through injection in a Class II brine disposal well (also called an injection well) because it requires little or no pretreatment and is often the cheapest management option (GAO 2012). This is not the case in the Marcellus Shale, where there are few Class II disposal wells. It may instead be cheaper to directly reuse wastewater, treat wastewater (onsite or offsite) for reuse, or treat wastewater for discharge. Injecting waste into disposal wells is an appealing option if wells are close, well capacity can handle wastewater volumes, disposal prices are low, and cheap, abundant fresh water is nearby (Karapataki 2012). In Pennsylvania, long travel distances to disposal wells and scarce water supplies have decreased the viability of injection disposal.

The Resource Conservation and Recovery Act allows for the disposal of oil and gas waste in Class II wells instead of the more stringently regulated Class I hazardous waste wells (Cooley et al. 2012). Class II wells include all three types of wells that accept fluids from oil and natural gas production: disposal wells, enhanced recovery wells, and hydrocarbon storage wells (EPA 2015a). All three types are regulated by EPA under the Underground Injection Control (UIC) well program, which requires that injection wells follow standards for construction and operation and imposes monitoring and reporting requirements to protect underground drinking water sources. The UIC program in Pennsylvania is administered by EPA. In Pennsylvania, injection well operators must first obtain an

UIC permit from EPA and a well permit from PADEP. Regulations require operators to monitor wellhead pressure to ensure that injection pressures do not surpass fracturing pressure. In 2014, Pennsylvania had more than 2,000 Class II wells but only eight active Class II disposal wells (Klapkowski 2014). This is because Marcellus geologic conditions are unfavorable for disposal wells and the two permits make the well approval process relatively difficult and expensive (Abdalla et al. 2011).

Given the lack of disposal wells in Pennsylvania, operators in Pennsylvania must transport brines to Ohio or West Virginia for disposal. Both states manage their own UIC programs and have more disposal wells than Pennsylvania. For 2011, Maloney and Yoxtheimer (2012) report that about 28 percent of brine water (produced water) was transported out of Pennsylvania to injection wells. Transportation to injection wells can be costly, upwards of \$100 an hour per truck (GE 2012) and operators must also pay disposal fees, which range in cost. And in July 2010, with the passage of Senate Bill 5, Ohio imposed a \$0.20 per barrel disposal fee for out-of-region waste (Braun 2015).

In addition to worries that wastewater injection may contaminate drinking water, concern has arisen that it may be responsible for increasing rates of seismic activity, at least in some geologic conditions. Whereas Arkansas, Colorado, New Mexico, Ohio, Oklahoma, Texas, and Virginia experienced an average total of 21 large earthquakes a year from 1967 to 2000, more 200 earthquakes were recorded in these states from 2010 to 2012, with 188 in 2011 (Ellsworth 2013). The recent increase in earthquake activity is illustrated below in Figure 4.

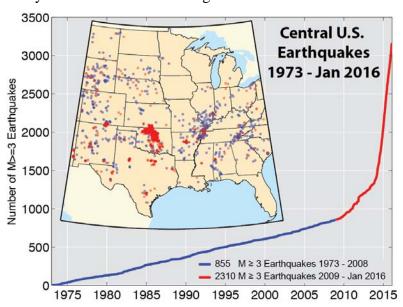


Figure 4. Central US Earthquakes, 1973-2015

Source: US Geological Survey, Earthquake Hazards Program, http://earthquake.usgs.gov/research/induced/

Earthquakes are considered induced by injection if they meet three criteria: proximity to injection wells, a change in background seismicity, and correlation with wastewater injection parameters (Keranen et al. 2013). However, using current seismological monitoring technology, it is impossible to distinguish between natural and induced seismic events with complete certainty (Folger and Tiemann 2014). Injecting fluids into the subsurface has been known to cause earthquakes by changing stresses in the earth's crust and pushing them out of equilibrium; this imbalance causes faults to slip (Folger and Tiemann 2014). Research has linked earthquakes in Ohio, Oklahoma, and other states to injection disposal (Keranen et al. 2013). Kim (2013) found that for earthquakes in 2011 and 2012 in Youngstown, Ohio, seismicity dropped when injection pressure and volumes decreased, indicating a link between injection and the 100 small earthquakes experienced in the area. The relationship between earthquake activity and the timing of injection, the amount and rate of waste fluid injected, local geologic conditions, and other factors is an area of ongoing research (Folger and Tiemann 2014). A recent study by Walsh and Zoback (2015) concluded that large volumes of highly saline water injected in a deep disposal zone of the Arbuckle formation led to rising pore pressure, which can penetrate already stressed basement faults and trigger earthquakes. Their study results were a major contributing factor in the recent statement from the Oklahoma Geological Survey that it was "very likely" that most of the state's recent earthquakes were due to the injection of produced water into disposal wells.

In response to increased evidence linking wastewater injection and induced seismicity, new regulations seek to reduce risks posed by injection practices. Following the 2011 earthquakes in Youngstown (Keranen et al. 2013), Ohio regulators reduced the number of permit approvals and tightened regulations, including limiting injection pressure and volumes for Class II wells (Schmidt 2013). As of 2014, both Pennsylvania and Ohio had limited wastewater injection pressure and volumes for Class II wells to limit damage and minimize risks from induced seismicity (GAO 2014). Going forward, more monitoring, disclosure, and perhaps even occasional moratoria may be among the tools regulators use to address this debated seismicity risk, with variations in requirements and enforcement priorities among states (Nicholson and Richards 2015).

# 2.7 Surface Water Discharge

Prior to 2011, operators in Pennsylvania could send their wastewater to publicly owned treatment works, but in 2011 PADEP requested that operators cease sending their wastewater to POTWs because they were incapable of cleaning wastewater to the desired standards (Zhang et al. 2016). POTWs, designed to handle municipal wastewater, could not adequately remove high levels of TDS and NORM from wastewater before discharging it into local rivers. Operators stopped shipping

waste to POTWs in January 2012 (Olmstead et al. 2013). For that reason, POTWs are excluded from our model (described in Section 4.3).

In 2010, PADEP promulgated new wastewater effluent standards for the natural gas industry that limit the monthly average concentrations of certain chemicals (EQB 2010): 500 mg/l for TDS, 250 mg/l for chlorides, 10 mg/l for barium, and 10 mg/l for strontium. The regulations apply to new or expanded facilities treating wastewater in Pennsylvania; 17 existing facilities are exempt from the regulation unless they wish to expand (EQB 2010). Currently, 25 newly proposed facilities are planning to treat natural gas wastewater for discharge to surface water by removing salts, metals, and oils and must meet the new TDS regulations.

Several published studies suggest that shale gas development may affect local surface water quality if water treatment plants have not sufficiently removed contaminants from the industry's wastewater. Olmstead et al. (2013), Warner et al. (2013), Ferrar et al. (2013), and Hladik et al. (2014) find evidence of high chloride, bromide, radium, barium, strontium, TDS, benzene, dibromochloronitromethane, and chloroform in surface water sources that receive effluent from facilities that treat wastewater from shale gas wells.

#### 2.8 Reclaimed Water Market and Beneficial Reuse

Revenue from fracking wastewater treatment, reuse, and recycling is anticipated to grow 30 percent annually and will reach \$3.8 billion by 2025 (Hardcastle 2016). Today, the produced water management market in the United States is estimated to be worth at least \$1.9 billion (Jerome 2015), thus creating many opportunities for innovative developments to lower the costs for transporting, storing, treating, and disposing of wastewater from fracking and obtaining water to drill and stimulate new wells. Operators need to evaluate the economics of managing water and wastewater, considering the costs of water acquisition, transport, and disposal. If well operators are unable to acquire the water supplies that they need, wells will underperform and lose money for operators (Brady 2014). In Pennsylvania, restricted disposal and treatment capacity and the high cost of water management have already led to several changes: increased reuse of wastewater, replacement of fresh water with brackish water, use of local and onsite water treatment, large wastewater management suppliers supporting multiple components of the water management process, changes in transportation practices,

<sup>&</sup>lt;sup>6</sup> Brady (2014) reports that as much as ten percent of capital expenditures and two thirds of operating expenses for shale wells can be associated with water management

(e.g., more reliance on pipes and onsite treatment to minimize trucking costs), and reduced disposal volumes (Gay and Slaughter 2014).

The costs of procuring and managing water used in oil and gas operations are huge and have created incentives for new approaches to handling shale gas wastewater. One company aiming to develop sustainable water management practices is Sourcewater, which has created a spot market for trading wastewater and reclaimed wastewater. The platform matches suppliers with operators and allows companies that offer trucking, treatment, storage, and disposal to post their services. The platform is not limited to those exclusively in the energy extraction industry; water rights owners, such as farmers, and utility companies can also supply or purchase water. In October 2015, after one year of operation, more than 100 companies were participating in the Sourcewater platform with some 1 billion barrels of water available for disposal, treatment, or reuse (Marcellus.com 2015). The price of water is a function of the quantity and quality of water. The system can improve the efficiency of water storage and transportation infrastructure and work better with the flexible schedules of water management, replacing inflexible contracts and commitments with a spot market (Marcellus.com 2015). According to Sourcewater (2014), if the market functions as designed, linking water and wastewater buyers, sellers and transporters, it will lower management costs, reduce risks of supply disruption, increase water recycling, decrease environmental risks, reduce transportation distances and costs, lower storage costs, reduce risks to human and environmental health, improve transaction speeds, and have other benefits for operators and the communities they operate in (Sourcewater 2014). Further, Sourcewater says its system will create incentives for investment in infrastructure to support a larger water commodities market and innovations required to meet future water needs (Sourcewater 2014).

As indicated by the scope of industries targeted to participate in Sourcewater's platform, the reclaimed water market includes many players and products that involve generating or buying wastewater, including some outside the shale gas industry. Other sources of demand that can be additional sources of revenue for wastewater treatment plants include injection for enhanced oil recovery (flooding) for nonshale areas, water service companies that provide water to well sites and

energy operators, industrial uses (power plant cooling, energy plant cooling, refineries), agriculture, road spreading, and resource recovery.<sup>7</sup>

# 3. Modeling Literature Review

Much of the literature on shale gas and water analyzes just one component of the water cycle (such as storage, transportation, treatment, disposal, or recycling), particularly with a focus on quantifying wastewater amounts, characterizing wastewater contaminant profiles, determining risks to drinking water supplies, and assessing and comparing treatment methods with respect to performance and cost. Several studies, described below, have developed models to optimize the wastewater management system (covering the storage, transportation, treatment and disposal of wastewater), but all differ, to a greater or lesser extent, from our model, which considers the industry's entire system of water procurement and wastewater management.

# 3.1 Wastewater Modeling Studies

Several recent papers deal with similar water management issues. Yang et al. (2014) developed a two-stage stochastic mixed-integer linear programming model to optimize the water-use life cycle for a well by minimizing transportation, treatment, storage, and disposal costs while accounting for revenue from gas production, creating an optimal fracturing schedule and recycling ratio. Their model assumes that well pad and treatment facility locations, freshwater sources, and river withdrawals are given and focuses on operational scheduling problems. Using their optimization model, they were able to reduce system operation costs, including trucking, disposal, and freshwater acquisition. They do not address the design capacities of the system components.

Yang et al. (2015) optimize capital investments to minimize the costs from freshwater acquisition and wastewater handling (including impoundment, piping, treatment facilities, and operation costs). They determine optimal impoundment capacity and location, pipe type, treatment

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<sup>&</sup>lt;sup>7</sup> Some pretreatment processes, such as Saltworks' ElectroChem Salt Splitter-RO system, have been able to produce gypsum from mining wastewater. This is done by mixing calcium ion and sulfate anions, which are normally separated into two different streams to reduce scaling issues. The mixing process forms gypsum which could be sold for profit. For more information, see (Frank 2016). Wastewater processing has yielded minerals and salts (including gypsum, iodine, lithium, NaCl) and acid base generation by-products and has been used for aquifer recharge and mining in some areas of the country (National Academies of Sciences 2016).

facility locations and removal capacity, freshwater sourcing, and frack schedules and test their mixed-integer linear programing model on a case study.

Gao and You (2015) model an optimized design and operation of a water supply chain network to maximize profit per unit of freshwater consumption and optimize performance and water-use efficiency. They include multiple transportation modes, management options, and treatment technologies. Their model allows for disposal, CWT, and onsite treatment. They analyze the optimal amount of water to be treated onsite for reuse and offsite at a CWT facility for recycling. Their model optimizes economic performance, which includes oil and gas production. With three tailored solution algorithms and two Marcellus case studies, they find that using pipeline to transport fresh water is more economic than using trucks; injection wells are not used for wastewater disposal because of high transportation costs. Furthermore, they find that more than 80 percent of wastewater is treated onsite; less than 20 percent is treated at a CWT facility and then discharged. Onsite treatment is preferred for meeting freshwater conservation, sustainable water flows, and reduced transportation.

Lira-Barragán et al. (2016) account for seasonal and environmental variation, such as variability in freshwater availability, as well as temporal changes in wastewater generation, to determine the optimal treatment, storage, reuse, and disposal options. They seek to minimize costs for freshwater acquisition, treatment, storage, disposal, and transportation while also minimizing the total annual costs of freshwater usage and wastewater discharge. They analyze the trade-offs between economics goals, such as cost minimization and system reliability (including the need to meet treatment and disposal requirements for flowback and produced water) as well as uncertainties involved in determining those trade-offs. The major contribution of their model is the consideration of the limitations associated with freshwater availability over different seasons. This is important because water availability affects the scheduling for well completion. Their case study results show that water reuse allows more wells to be completed, each using less fresh water at a lower cost.

In addition to the literature described above, several online water management decision tools and optimization models exist. However, all of these studies and tools use assumptions and conditions that limit the usefulness of the optimization model results, and they lack an analysis or discussion of the sale of reclaimed water in the water reuse market. In addition, each model is unable to encompass the full range of treatment and disposal options and include all components of the shale gas system. None explicitly account for externalities or focus on multiple decisionmakers.

## 3.2 Differences between Our Model and Existing Work

Our model is different from those described in the previous section in the following ways.

- Our model focuses much more on the wastewater reuse component of wastewater management.
- Our model considers four decisionmakers: oil and gas well developers and operators, centralized wastewater treatment facility planners and operators, environmental regulators, and social planners. The above studies do not include social planners or consider the regulatory component as a constraint.
- Our paper considers both water balance and chemical mass balance of water throughout all
  periods of shale gas development and throughout the entire life cycle of water used in shale gas
  production. This allows us to consider water quality requirements for water reuse and pollutant
  effluent discharge as well as the influent water quality requirements of treatment technologies.
  All water quality constraints are represented as a concentration (ppm), which requires
  knowledge of both pollutant mass and water quantity. Most previous research considers only
  water balance, not pollutant mass balance.
- Our modeling framework incorporates more environmental externalities than other papers and considers social welfare. Other work optimizes environmental effects in relation to water withdrawal levels and water-use efficiency. Our modeling framework includes truck emissions, both CO<sub>2</sub> and conventional air pollutants; population exposure to transportation accidents and spills; solid waste generation; and induced seismicity from deep well injection. We model social impacts associated with water and wastewater management much more explicitly.
- Our modeling framework includes a reclaimed water market. The market provides different
  reclaimed water market prices based on the quality of the reclaimed water. A reclaimed water
  market can provide a source of revenue for CWT facilities and another source of water for well
  operators.

We hope to develop a comprehensive modeling and optimization framework for integrated design and operation of shale gas water and wastewater management with explicit consideration of

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<sup>&</sup>lt;sup>8</sup> We plan to include road damage from water and wastewater trucking in future work.

management options, including both private and social costs. Our current model does have limitations, for tractability. In particular, because we track the concentration of pollutants at every component of the modeling system, we have formulated a nonlinear and nonseparable mathematical programming problem that is very difficult to solve using commercial mathematical optimization packages.

# 4. Model Development

Water and wastewater management in shale gas development is a highly complicated issue. We investigate the life cycle of water and wastewater management processes and adopt a holistic systems approach for our analysis. We aim to develop a decision-support framework: a multi-objective dynamic optimization model for integrated shale gas water, wastewater, and solid waste management.

# 4.1 System Domain

Figure 5 shows our study domain. The entire system includes 14 components: well pads (P), freshwater sources (F), wells (W), storage for onsite flowback and produced water (S1), storage for onsite reclaimed water (S2), storage for centralized wastewater (S3), storage for centralized reclaimed water (S4), an onsite wastewater treatment facility (OW), a centralized wastewater treatment plant (CW), deep well injection (D), surface water discharge (R), other (not shale well) demand for reclaimed water (OD), and a landfill site for solid waste disposal (LF). These components are connected by arrows of different colors. Blue arrows represent freshwater flow; black, wastewater flow; purple, reclaimed water flow; and orange, solid waste shipment. For every component and link, the water and chemical mass balances are maintained. Dashed lines indicate transportation-relevant environmental externalities, such as emissions of CO<sub>2</sub> and conventional air pollutants, road damage, crashes, and contamination exposure due to road spills. Dashed boxes at the deep injection well reflect seismicity risk associated with wastewater injection.

<sup>&</sup>lt;sup>9</sup> In this study, TDS is the only chemical we consider. We plan to add at least one more toxic chemical in the future.

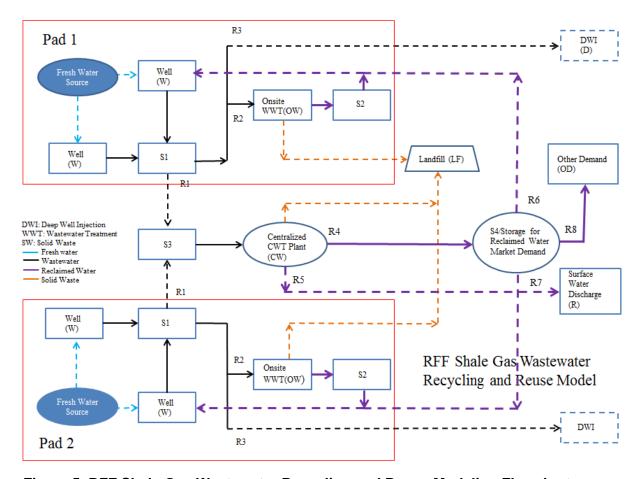


Figure 5. RFF Shale Gas Wastewater Recycling and Reuse Modeling Flowchart

We assume that the quantity of available fresh water, water demand, wastewater generation schedules at individual wells, and other demands for reclaimed water in the system domain are known by the well operator. For every well, the water demand for hydraulic fracturing at a predetermined schedule is met by water from three sources: fresh water, onsite reclaimed water, and offsite or centralized reclaimed wastewater. The water mixture must be of the quality required for hydraulic fracturing of the particular well. Other reclaimed wastewater sources, such as municipal wastewater, are not considered now but could be included in the future.

 $<sup>^{10}</sup>$  We will relax this assumption and consider uncertainty associated with the system parameters and input data in the future.

# 4.2 Model Objective and Constraints

The multi-objective programming model has four decisionmakers, as noted above. For well developers and operators, the objective is to minimize water and wastewater management costs, including water acquisition, transportation, onsite wastewater storage, <sup>11</sup> onsite wastewater treatment, and offsite wastewater and solid waste treatment and disposal. For CWT facility planners and operators, the objective is to minimize the capital and O&M costs of their facility and maximize the revenue from selling reclaimed water and other recovered resources. O&M costs are influenced by the need to store influent water, the chemical profile of the influent water, and the treatment technology (and its associated energy costs). Sources of revenue for CWT facilities are selling reclaimed water to well operators for fracking, selling reclaimed water for other beneficial uses, and selling other recovered resources. We assume that the destination of water intended for beneficial reuse is close to the CWT facility, and accordingly, transportation costs to deliver the reclaimed water and/or recovered resources from the CWT facility to beneficial reusers can be ignored. 12 For environmental regulators, the objective is to minimize environmental harms and ensure enforcement of relevant laws. In our model, the regulators will focus on emissions of CO<sub>2</sub> and conventional air pollutants, solid waste generation, seismological risks, surface water contamination from CWT facility effluent, and population exposure to traffic accidents and chemical spills. This list of environmental externalities is by no means complete; we use it to demonstrate the model's capability but do not include all externalities because of the significant uncertainty about many risk pathways associated with shale gas operations. Social planners aim to minimize social costs—both private costs and environmental externalities—and therefore consider the system design and operations from a combination of the previous three decisionmakers' perspectives.

The decision variables include the treatment capacity of onsite wastewater treatment facilities at an individual well pad, the treatment capacity of centralized wastewater treatment plants, onsite storage capacity, wastewater allocations to the various management options (deep well injection, onsite treatment, offsite treatment), treatment technologies and levels (primary, secondary, tertiary), and reclaimed water allocations between surface discharge and reuse via the reclaimed water market. For onsite treatment and CWT facilities, up to three treatment technologies and levels are considered.

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<sup>&</sup>lt;sup>11</sup> Wastewater storage is important to consider before wastewater treatment because of the intermittent flow of wastewater and high variability of the pollutant concentration. Storage could reduce wastewater treatment design capacity and improve the performance of the wastewater treatment technology.

<sup>&</sup>lt;sup>12</sup> We will also relax this assumption in the future.

For wastewater treatment technologies, the removal efficiency at every facility can be different; efficiency rates are provided by the model user. The decision variables at the treatment facility include the design capacity of the treatment technology and the quantity of wastewater to be treated with that technology option. The model inputs include variations in fracking water demand, wastewater generation rates, chemical profiles, reclaimed water demand for other beneficial reuse over time, and other economic and noneconomic parameters.

## 4.3 Wastewater Management Options

Currently, well operators have several wastewater management options (Figure 5). For this model we use the following options:

- Onsite blending without treatment. This is followed by recycling and reuse to frack a
  subsequent well. Wastewater recycling and reuse reduce freshwater acquisition and
  transportation costs. It is often the cheapest wastewater management option, but the operator
  incurs a risk of well plugging, equipment damage, and reduced gas production.
- Onsite treatment using a mobile treatment unit. This can include primary, secondary, and/or tertiary treatment and involve several types of technologies, which will influence the cost of treatment and the quality of the treated water. Costs are generally modest or high. The major shortcoming of onsite treatment is limited treatment capacity. For this model, we consider three treatment technologies (representing different treatment levels) for onsite treatment:

Technology 1: Primary

Technology 2: Primary + secondary

Technology 3: Primary + secondary + tertiary

• Treatment at an offsite centralized wastewater treatment facility for surface water discharge. CWT facilities may treat water for reuse in fracking or other beneficial uses or may treat water for release. In 2010 PADEP established effluent discharge standards of 500 ppm of TDS and 250 ppm of chloride, along with other restrictions. Some industrial wastewater treatment plans that handle oil and gas wastewater are exempt from these standards, but their capacities are limited. Currently, 25 proposed CWT plants and others that are not exempt from the 2010 regulations will likely need to adopt advanced tertiary treatment methods, such as thermal distillation, crystallization, or vacuum evaporation, to meet the stringent effluent discharge standards. For our model, we assume that offsite treatment involves tertiary treatment to the desired water quality standard, either for discharge or for reuse.

- Offsite centralized wastewater treatment for fracking and other beneficial reuse. Some
  treatment processes can yield relatively high quality water that could be recycled for fracking
  or used outside the oil and gas industry. The water quality of the end product depends on the
  method of reuse; for some uses, the water quality requirements may be less stringent than
  surface discharge standards. In this model, the wastewater could receive tertiary treatment for
  surface water discharge or could be treated to a lower quality, depending on the specific
  beneficial use.
- Onsite storage followed by transportation to Class II disposal wells for underground or deep well injection. Our model considers disposal wells only and does not consider other types of Class II injection wells.

Each treatment technology has different capital costs, variable costs, pollutant concentration removal rates, wastewater loss (recovery) rates, and solid waste generation potential. For each component and link, we keep track of both the water balance and the pollutant mass balance. This allows us to estimate the onsite reclaimed water quantity and effluent pollutant concentration for each treatment option. If the effluent is discharged to surface water, the pollutant concentration needs to be in compliance with the effluent discharge standards set by PADEP. When reclaimed water is blended with fresh water to prepare fracking fluid, the pollutant concentration in the mixing water has to meet the water quality requirement specified by the operator.

Wastewater is stored onsite on a per well pad basis using ponds and/or tanks. Onsite storage is necessary because the amount of flowback and produced wastewater varies over time, and the onsite treatment capacity is limited and may be insufficient during periods of peak wastewater generation. The peak generation of flowback and produced wastewater occurs just after the hydraulic fracturing pressure is released; generation then gradually declines over the lifetime of the well. Storage options can reduce the peak design capacity of the onsite wastewater treatment facility and, hence, reduce the capital investment cost.

Wastewater stored onsite can be treated and/or disposed of using one of three options. First, it can be sent to a deep injection well for disposal, which involves high transportation costs, as well as the fee charged by the injection well operator. Second, it can be treated and reclaimed onsite and stored for onsite reuse. Onsite treatment facilities usually have limited treatment capacity, technology, and efficiency and may be more expensive because they lack economies of scale. Third, it can be shipped offsite to a CWT facility for treatment. CWT facilities have the advantage of economies of scale and can recover other resources in the process of cleaning the water, but using a CWT plant may involve high transportation costs. The effluent from CWT plants can be stored and sold in the reclaimed water market, for reuse in either oil and gas well development or other industries, or it can

be sent to surface water for discharge if it has been sufficiently treated to meet effluent discharge standards.

# 4.4 The Model

In this section, we discuss a modeling framework for evaluating hydraulic fracturing wastewater management options. We first provide the definitions of the notation used in Figure 5 and the model:

#### **Indices**

f	freshwater source index
p	well pad index
$\overline{w}$	well index
l	landfill site index
c	centralized wastewater treatment (CWT) facility index
d	deep well index
i	wastewater treatment technology index
j	pollutant index
t	time period index, in weeks or days

# **Nodes and components**

$\boldsymbol{F}$	freshwater source
W	well
<i>S1</i>	onsite pit and pond or tank storage
<i>S</i> 2	storage for onsite reclaimed water
<i>S3</i>	influent storage at individual centralized wastewater treatment plant
<i>S4</i>	storage for CWT reclaimed water and for reclaimed water market
OW	onsite wastewater treatment
L	landfill
D	deep well injection
CW	centralized wastewater treatment plant
R	surface water or river discharge
OD	other reuse of reclaimed water
EF	transportation emissions factor
MRF	material recovery factor

# Water and wastewater links

$F_W_{f,w,p,t}$	Fresh water from water source $f$ to well $w$ in pad $p$ , during time period $t$ .
$W_{\_}SI_{w,p,t}$	Flow from well w to storage S1 in pad p, during time period t.
$S1\_D_{p,d,t}$	Flow from storage S1 in pad p to deep well d, during time period t.

Flow from storage S1 to OW in pad p, during time period t.  $SI OW_{i,p,t}$ 

Flow from storage S1 in pad p to centralized storage S3, during time period t.  $S1 S3_{p,c,t}$ 

 $OW_S2_{i,p,t}$ Flow from OW to storage S2 in pad p, during time period t.

Flow of reclaimed water from storage S2 to well W in pad p, during time period t.  $S2 W_{w,p,t}$ 

Flow from centralized storage S3 to CW, during time period t.  $S3\_CW_{i,c,t}$ 

Flow from CW to storage S4, during time period t. CW  $S4_{i,c,t}$ 

Flow from CW to river discharge R, during time period t.  $CW_R_{i,c,t}$ 

 $S2\_R_{p,t}$ Reclaimed water from S2 in pad p, sent to river R to discharge, during time period t.

 $S2\_S4_{p,c,t}$ Onsite reclaimed water from storage S2 in pad, p, sent to S4 for reclaimed water

market demand storage, during time period t.

S4  $D_{c,d,t}$ Reclaimed water sent from reclaimed water market demand storage, S4, to deep well

D, during time period t.

Reclaimed water sent from reclaimed water market demand storage, S4, to river for  $S4 R_{c,t}$ 

discharging, during time period t.

Reclaimed water sent from reclaimed water market demand storage, S4, to well W,  $S4\_W_{c,p,t}$ 

in pad P, during time period t.

 $S4\_OD_{c,t}$ Reclaimed water sent from reclaimed water market demand storage, S4, to other

market demand OD, during time period t.

#### **Solid waste links**

 $OW\_LF_{i,p,l,t}$ : Solid waste sent from OW at pad, p, to landfill, LF, l, during time period t.

CW  $LF_{i,c,l,t}$ : Solid waste sent from CW to landfill L, during time period t.

#### 4.4.1 Variables

The variable with "q" in front of a link is a water flow variable. The variable with a "c" in front of a link is a concentration variable. The variable with an "s" in front of a link is a solid waste variable. The variable with a "d" in front of a link is a distance parameter. The variable with a "p" in front of a link is a population parameter along the link. For example,  $q_F W_{f,w,p,t}$  represents the quantity of water shipped from freshwater source f to well w in pad p during time period t.  $c_F W_{f,w,p,t}$  represents the pollutant concentration in the water.  $d_F W_{f,w,p,t}$  represents the distance of the water source f and well pad p, and  $p_F = W_{f,w,p,t}$  represents population along water source f and well pad p.

**Table 1. Summary of Variables** 

		Concentration	
	Flow variable	variable for each	Distance
	for each link	link and state	variable
Link	(gal/week)	variable (ppm)	(mile)
$F_{-}W_{f,w,p,t}$	$q_F_W_{f,w,p,t}$	$c_F_W_{f,w,p,t}$	$d_F_W_{f,p}$
$W_SI_{w,p,t}$	$q_W_SI_{w,p,t}$	$c_W_SI_{w,p,t}$	
$SI\_D_{p,d,t}$	$q\_S1\_D_{p,d,t}$	$c\_SI\_D_{p,d,t}$	$d\_S1\_D_{p,d}$
$S1\_OW_{i,p,t}$	$q_S1_OW_{i,p,t}$	$c\_SI\_OW_{i,p,t}$	

$S1\_S3_{p,c,t}$	$q\_S1\_S3_{p,c,t}$	$c\_S1\_S3_{p,c,t}$	$d\_S1\_S3_{p,c}$
$OW\_S2_{i,p,t}$	$q_OW_S2_{i,p,t}$	$c\_OW\_S2_{i,p,t}$	
$S2\_W_{w,p,t}$	$q\_S2\_W_{w,p,t}$	$c\_S2\_W_{w,p,t}$	
$S2\_D_{p,d,t}$	$q\_S2\_D_{p,d,t}$	$c\_S2\_D_{p,d,t}$	$d\_S2\_D_{p,d}$
$S3\_CW_{i,c,t}$	$q_S3_CW_{i,c,t}$	$c_S3_CW_{i,c,t}$	
$CW\_S4_{i,c,t}$	$q_CW_S4_{i,c,t}$	$c\_CW\_S4_{i,c,t}$	
$CW\_R_{i,c,t}$	$q_CW_R_{i,c,t}$	$c\_CW\_R_{i,c,t}$	$d_CW_R_c$
$S2\_R_{p,t}$	$q\_S2\_R_{p,t}$	$c\_S2\_R_{p,t}$	$d\_S2\_R_p$
$S2\_S4_{p,c,t}$	$q_S2_S4_{p,c,t}$	$c\_S2\_S4_{p,c,t}$	$d_S2_S4_{p,c}$
$S4\_D_{c,d,t}$	$q\_S4\_D_{c,d,t}$	$c\_S4\_D_{c,d,t}$	$d\_S4\_D_{c,d}$
$S4\_R_{c,t}$	$q\_S4\_R_{c,t}$	$c\_S4\_R_{c,t}$	$d\_S4\_R_c$
$S4\_W_{c,p,w,t}$	$q\_S4\_W_{c,p,w,t}$	$c\_S4\_W_{c,p,w,t}$	$d\_S4\_W_{c,p}$
$S4\_OD_{c,t}$	$q\_S4\_OD_{c,t}$	$c\_S4\_OD_{c,t}$	$d\_S4\_OD_c$
$OW\_LF_{i,p,l,t}$	$s\_OW\_LF_{i,p,l,t}$		$d_OW_LF_{p,l}$
$CW\_LF_{i,c,l,t}$	$s\_CW\_LF_{i,c,l,t}$		$d_CW_LF_{c,l}$

State variable	Concentration of
(gal)	state variable (ppm)
$SI_{p,t}$	$c\_SI_{p,t}$
$S2_{p,t}$	$c\_S2_{p,t}$
$S3_{c,t}$	$c\_S3_{c,t}$
$S4_{c,t}$	$c\_S4_{c,t}$

Decision variables	
$cap\_OW_{i,p}$	Design treatment capacity for onsite wastewater treatment technology <i>i</i> , gal/week
$cap\_CW_{i,c}$	Design treatment capacity for CWT facility using technology i, gal/week
$cap\_SI_p$	Design impoundment storage capacity for onsite wastewater treatment at pad p, gal
$cap \_S2_p$	Design impoundment storage capacity for onsite reclaimed water at pad p, gal
cap_S3 <sub>c</sub>	Design storage capacity for influent of CWT plant, gal
cap_S4c	Design storage capacity for CWT plant reclaimed water, gal
$cap\_tank1_p$	Design tank storage capacity for onsite wastewater treatment at pad p, gal
cap_tank2 <sub>p</sub>	Design tank storage capacity for onsite reclaimed water at pad p, gal, gal
$RI_{p,t}$	Wastewater allocation to CWT plant at pad p, during time period t, %
$R2_{p,t}$	Wastewater allocation to onsite wastewater treatment facility at pad <i>p</i> , during time period <i>t</i> , %
$R3_{p,t}$	Wastewater allocation to deep well injection at pad <i>p</i> , during time period <i>t</i> , %
$R4_{c,t}$	CWT reclaimed water allocated to reclaimed water market storage during time period t, %
$R5_{c,t}$	CWT reclaimed water allocated to surface water discharge, during time period t, %
$R6_{c,w,p,t}$	Reclaimed water returns to well w at pad p during t for fracking, %
$R7_{c,w,p,t}$	Reclaimed water returns to well w at pad p during time period t for fracking, %
$R8_{c,t}$	Reclaimed water sold to other demand during time period t, %
$y_c$	CWT opening variable, a binary variable; 1 if CWT c is opened; 0 otherwise

# Table 2. Model Inputs

Noncost inputs		
$WD_{w,p,t}$	Water demand profile at well $w$ , pad $p$ and time period $t$ , gal/week	
TDS_limit	TDS concentration limit in the water preparing for HF, ppm	
$WWG_{w,p,t}$	Flowback and produced wastewater generation profile from well $w$ , pad $p$ and time period $t$ ,	
	gal/week	
$conc\_WWG_{w,p,t}$	Pollutant (TDS) concentration profile in FP wastewater stream, ppm	
sw_factor <sub>i</sub>	Technology <i>i</i> specific solid waste generation factor	
$r\_OW_{i,p}$	Pollutant removal efficiency at the onsite wastewater treatment technology $i$ , at pad $p$ , %	
$r\_CW_{i,c}$	Pollutant removal efficiency at the CWT plant, C, using treatment technology i, %	
$EF_j$	Polluatnt j emissions factor, g/bbl-mile or g/ton-mile	

$cap\_LF_1$ Solid waste disposal capacity at landfill site $l$ , tons/week $d\_F\_W_{fp}$ Distance between freshwater source $f$ and well $w$ in pad $p$ , mile $d\_SI\_D_{p,d}$ Distance between $SI$ in pad $p$ and deep well $d$ , mile $d\_SI\_D_{p,d}$ Distance between $SI$ in pad $p$ and deep well $d$ , mile $d\_SU\_D_{p,d}$ Distance between $SI$ in pad $p$ and deep well $d$ , mile $d\_CW\_Rc$ Distance between CWT and location for surface water discharge, mile $d\_SU\_R_p$ Distance between $SI$ in pad $p$ and location for surface water discharge, mile $d\_SU\_R_p$ Distance between $SI$ in pad $p$ and $I$ in $I$ i	_	
$dFW_{fp}$ Distance between freshwater source $f$ and well $w$ in pad $p$ , mile $dSID_{p,d}$ Distance between $SI$ in pad $p$ and deep well $d$ , mile $dSID_{p,d}$ Distance between $S2$ in pad $p$ and $S3$ , mile $dSID_{p,d}$ Distance between $S2$ in pad $p$ and deep well $d$ , mile $dCWRc$ Distance between $S2$ in pad $p$ and location for surface water discharge, mile $dSISID_{p,c}$ Distance between $S2$ in pad $p$ and location for surface water discharge, mile $dSISID_{p,c}$ Distance between $SIDDDDDDDDDDDDD_$	$cap\_D_d$	Injection/disposal capacity at deep well d, gal/week
$d\_SI\_D_{p,d}$ Distance between $SI$ in pad $p$ and deep well $d$ , mile $d\_SI\_S3_{p,c}$ Distance between $S2$ in pad $p$ and $p$ and deep well $d$ , mile $d\_S2\_D_{p,d}$ Distance between $S2$ in pad $p$ and location for surface water discharge, mile $d\_SZ\_R_p$ Distance between $SZ$ in pad $p$ and location for surface water discharge, mile $d\_SZ\_R_p$ Distance between $SZ$ in pad $p$ and $SZ$ , mile $d\_SZ\_A_{p,c}$ Distance between $SZ$ in pad $p$ and $SZ$ , mile $d\_SZ\_A_{p,c}$ Distance between $SZ$ and deep well $d$ , mile $d\_SZ\_A_{p,c}$ Distance between $SZ$ and location for surface water discharge, mile $d\_SZ\_D_{p,c}$ Distance between $SZ$ and location for other demand of reclaimed water, mile $d\_SZ\_D_{p,c}$ Distance between $SZ$ and location for other demand of reclaimed water, mile $d\_D_{p,c}$ Distance between onsite wastewater treatment at pad $p$ and landfill site $l$ , mile $d\_CM\_LF_{p,l}$ Distance between onsite wastewater treatment at pad $p$ and landfill site $l$ , mile $p\_F\_M_{l,p}$ Population exposure between freshwater source $f$ and well $w$ in pad $p$ , mile $p\_SI\_D_{p,d}$ Population exposure between $SZ$ in pad $p$ and deep well $d$ , mile $p\_SI\_D_{p,d}$ Population exposure between $SZ$ in pad $p$ and deep well $d$ , mile $p\_SZ\_D_{p,c}$ Population exposure between $SZ$ in pad $p$ and location for surface water discharge, mile $p\_SZ\_D_{p,c}$ Population exposure between $SZ$ in pad $p$ and location for surface water discharge, mile $p\_SZ\_D_{p,c}$ Population exposure between $SZ$ in pad $p$ and $SZ$ , mile $p\_SZ\_D_{p,c}$ Population exposure betw	cap_LF <sub>l</sub>	Solid waste disposal capacity at landfill site <i>l</i> , tons/week
$d\_SI\_S3_{p,c}$ Distance between $S2$ in pad $p$ and $S3$ , mile $d\_S2\_D_{p,d}$ Distance between $S2$ in pad $p$ and deep well $d$ , mile $d\_SZ\_R_p$ Distance between $S2$ in pad $p$ and location for surface water discharge, mile $d\_SZ\_S4_{p,c}$ Distance between $S2$ in pad $p$ and $S4$ , mile $d\_S4\_D_{c,d}$ Distance between $S4$ and deep well $d$ , mile $d\_S4\_D_{c,d}$ Distance between $S4$ and deep well $d$ , mile $d\_S4\_D_{c,d}$ Distance between $S4$ and location for surface water discharge, mile $d\_S4\_W_{c,p}$ Distance between $S4$ and location for other demand of reclaimed water, mile $d\_S4\_D_{c,d}$ Distance between $S4$ and location for other demand of reclaimed water, mile $d\_CW\_LF_{p,l}$ Distance between onsite wastewater treatment at pad $p$ and landfill site $l$ , mile $d\_CW\_LF_{c,l}$ Distance between CWT and landfill site $l$ , mile $p\_S1\_D_{p,d}$ Population exposure between freshwater source $f$ and well $w$ in pad $p$ , mile $p\_S1\_D_{p,d}$ Population exposure between $S1$ in pad $p$ and deep well $d$ , mile $p\_S2\_D_{p,d}$ Population exposure between $S2$ in pad $p$ and deep well $d$ , mile $p\_S2\_D_{p,d}$ Population exposure between $S2$ in pad $p$ and location for surface water discharge, mile $p\_S2\_S4_{p,c}$ Population exposure between $S2$ in pad $p$ and location for surface water discharge, mile $p\_S4\_D_{c,d}$ Population exposure between $S4$ and deep well $d$ , mile $p\_S4\_D_{c,d}$ Population exposure between $S4$ and location for surface water discharge, mile $p\_S4\_D_{c,d}$ Population exposure between $S4$ and location for surface water disch	$d_F_W_{f,p}$	Distance between freshwater source $f$ and well $w$ in pad $p$ , mile
$d\_S2\_D_{p,d}$ Distance between S2 in pad $p$ and deep well $d$ , mile $d\_CW\_R_c$ Distance between CWT and location for surface water discharge, mile $d\_S2\_R_p$ Distance between S2 in pad $p$ and location for surface water discharge, mile $d\_S2\_S4_{p,c}$ Distance between S2 in pad $p$ and S4, mile $d\_S4\_D_{c,d}$ Distance between S4 and deep well $d$ , mile $d\_S4\_D_{c,d}$ Distance between S4 and location for surface water discharge, mile $d\_S4\_D_{c,p}$ Distance between S4 and well $w$ in pad $p$ , mile $d\_S4\_D_{c,p}$ Distance between S4 and location for other demand of reclaimed water, mile $d\_OW\_LF_{p,l}$ Distance between Outrand landfill site $l$ , mile $d\_CW\_LF_{c,l}$ Distance between CWT and landfill site $l$ , mile $p\_F\_W_{lp}$ Population exposure between freshwater source $f$ and well $w$ in pad $p$ , mile $p\_S1\_D_{p,d}$ Population exposure between S2 in pad $p$ and deep well $d$ , mile $p\_S1\_S3_{p,c}$ Population exposure between S2 in pad $p$ and deep well $d$ , mile $p\_S2\_D_{p,d}$ Population exposure between S2 in pad $p$ and location for surface water discharge, mile $p\_S2\_D_{p,d}$ Population exposure between S2 in pad $p$ and location for surface water discharge, mile $p\_S2\_R_p$ Population exposure between S2 in pad $p$ and location for surface water discharge, mile $p\_S4\_D_{c,d}$ Population exposure between S4 and location for surface water discharge, mile $p\_S4\_R_c$ Population exposure between S4 and location for surface water discharge, mile $p\_S4\_R_c$ Population exposure between S4 and location for other demand of reclaimed water, mile		Distance between $SI$ in pad $p$ and deep well $d$ , mile
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$d\_S2\_R_p$ Distance between $S2$ in pad $p$ and location for surface water discharge, mile $d\_S2\_S4_{p,c}$ Distance between $S2$ in pad $p$ and $S4$ , mile $d\_S4\_D_{c,d}$ Distance between $S4$ and deep well $d$ , mile $d\_S4\_R_c$ Distance between $S4$ and location for surface water discharge, mile $d\_S4\_W_{c,p}$ Distance between $S4$ and well $w$ in pad $p$ , mile $d\_S4\_DD_c$ Distance between $S4$ and location for other demand of reclaimed water, mile $d\_OW\_LF_{p,l}$ Distance between onsite wastewater treatment at pad $p$ and landfill site $l$ , mile $d\_CW\_LF_{p,l}$ Distance between CWT and landfill site $l$ , mile $p\_F\_W_{f,p}$ Population exposure between freshwater source $f$ and well $w$ in pad $p$ , mile $p\_S1\_Dp_{p,d}$ Population exposure between $S1$ in pad $p$ and deep well $d$ , mile $p\_S1\_S3_{p,c}$ Population exposure between $S2$ in pad $p$ and deep well $d$ , mile $p\_S2\_Dp_{p,d}$ Population exposure between $S2$ in pad $p$ and location for surface water discharge, mile $p\_S2\_R_p$ Population exposure between $S2$ in pad $p$ and location for surface water discharge, mile $p\_S2\_S4_{p,c}$ Population exposure between $S2$ in pad $p$ and $S3$ , mile $p\_S4\_Dc_{c,d}$ Population exposure between $S4$ and deep well $d$ , mile $p\_S4\_Dc_{c,d}$ Population exposure between $S4$ and deep well $d$ , mile $p\_S4\_Dc_{c,d}$ Population exposure between $S4$ and location for surface water discharge, mile $p\_S4\_Dc_{c,d}$ Population exposure between $S4$ and location for other demand of reclaimed water, mile $p\_S4\_Dc_{c,p}$ Population exposure between $S4$ and location	$d\_S2\_D_{p,d}$	Distance between $S2$ in pad $p$ and deep well $d$ , mile
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Distance between S4 and deep well d, mile  Distance between S4 and location for surface water discharge, mile  Distance between S4 and location for other demand of reclaimed water, mile  Distance between S4 and location for other demand of reclaimed water, mile  Distance between onsite wastewater treatment at pad p and landfill site l, mile  Distance between onsite wastewater treatment at pad p and landfill site l, mile  Distance between CWT and landfill site l, mile  PF_Wf_p  Population exposure between freshwater source f and well w in pad p, mile  P_S1_Dp_d  Population exposure between S1 in pad p and deep well d, mile  P_S1_S3_p,c  Population exposure between S2 in pad p and deep well d, mile  P_S2_Dp_d  Population exposure between S2 in pad p and location for surface water discharge, mile  P_S2_Rp  Population exposure between S2 in pad p and location for surface water discharge, mile  P_S2_S4_p,c  Population exposure between S2 in pad p and S4, mile  P_S4_Dc_d  Population exposure between S4 and deep well d, mile  P_S4_Pc_d  Population exposure between S4 and deep well d, mile  P_S4_Dc_d  Population exposure between S4 and location for surface water discharge, mile  P_S4_Wc_p  Population exposure between S4 and location for surface water discharge, mile  P_S4_Dc_d  Population exposure between S4 and location for surface water discharge, mile  P_S4_Dc_d  Population exposure between S4 and location for surface water discharge, mile  P_S4_Dc_d  Population exposure between S4 and location for other demand of reclaimed water, mile  P_OW_LF_{p,l}  Population exposure between OWT and landfill site l, mile  P_CW_LF_{p,l}  Population exposure between CWT and landfill site l, mile	$d_S2R_p$	Distance between S2 in pad p and location for surface water discharge, mile
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$p\_CW\_LF_{c,l}$ Population exposure between CWT and landfill site $l$ , mile	$p\_S4\_OD_c$	
	$p\_OW\_LF_{p,l}$	Population exposure between onsite wastewater treatment at pad $p$ and landfill site $l$ , mile
$p_F - W_{f,p}$ Population exposure between freshwater source f and well w in pad p, mile	$p\_CW\_LF_{c,l}$	Population exposure between CWT and landfill site <i>l</i> , mile
	$p_F_W_{f,p}$	Population exposure between freshwater source $f$ and well $w$ in pad $p$ , mile

Cost inputs	
tanktruckcost	Tank truck transportation cost, \$/gal-mile
pipecost	Pipe water transportation cost, \$/gal-mile
truckcost	Truck transportation cost, \$/ton/mile, for shipping solid waste or hazardous materials
capcost_OWi	Capital cost of onsite treatment technology <i>i</i> , \$/gal
capcost_CW <sub>i</sub>	Capital cost of centralized treatment technology <i>i</i> , \$/gal
capcost_S1	Capital cost of onsite storage S1, either impoundment or tank storage, \$/gal
capcost_S2	Capital cost of onsite storage S2, either impoundment or tank storage, \$/gal
capcost_S3	Capital cost of onsite storage S3, either impoundment or tank storage, \$/gal
capcost_S4	Capital cost of onsite storage S4, either impoundment or tank storage, \$/gal
omcost_OWi	O&M cost of onsite treatment technology <i>i</i> , as a function of flow, \$/gal
omcost_CWi	O&M cost of CWT treatment technology i, as a function of flow, \$/gal
omcost_tank	O&M cost of onsite tank storage, \$/gal
omcost_D	Deep well injection cost, \$/gal
omcost_LF	Landfill tipping fee, \$/ton

# **4.1.2** Water Balance Constraints

At every well W, the specified water demand for well w in pad p, during time period t,  $WD_{w,p,t}$ , will include fresh water,  $q_F W_{w,p,t}$ , reclaimed water from onsite treatment,  $q_S 2 W_{w,p,t}$ , and reclaimed

water purchased from reclaimed water market,  $q_S4_W_{w,p,t}$ .  $WD_{w,p,t}$  in bold means that the water demand is provided by the model user or well developer, based on the hydraulic fracturing schedule.

$$\sum_{f} q_{-}F_{-}W_{f,w,p,t} + q_{-}S2_{-}W_{w,p,t} + q_{-}S4_{-}W_{w,p,t} = WD_{w,p,t} , \forall w, p,t$$
 (1)

At every well W, the wastewater flow from well W to storage SI in pad p, during time period t, is equal to the amount of wastewater (flowback and produced water) generated from well w in pad p, during time period t,  $WWG_{w,p,t}$ . We assume that the operator is aware of the wastewater generation profile and schedule. In the future we will relax this assumption and consider uncertainties in wastewater generation.

$$q_{W} S1_{w,p,t} = WWG_{w,p,t} \quad \forall w, p, t$$
 (2)

The onsite wastewater storage  $SI_{p,t}$  at pad p during time period t is equal to the storage at the end of the previous time period plus all the inflows minus all the outflows during this time period. The inflow streams include wastewater generated from all the wells in pad p during time period t. Outflow streams include wastewater sent to Class II injection well D for disposal, sent offsite to a CWT facility for treatment and treated onsite.

$$S1_{p,t} = S1_{p,t-1} + \sum_{w} q_{w} - S1_{w,p,t} - \sum_{d} q_{w} - S1_{w} - \sum_{d} q_{w} - \sum_{d} q_{w}$$

We assume that storage,  $SI_{p,t}$ , at any time should be less than or equal to the storage design capacity and satisfies the following design capacity constraint:

$$S1_{p,t} \le cap \_S1_p , \forall p,t \tag{4}$$

We assume that there is no water loss for onsite wastewater treatment. Wastewater is split between two outflow streams: (1) onsite wastewater treatment plant followed by posttreatment storage, then reuse; and (2) onsite wastewater treatment followed by transportation to a landfill. For simplicity, we assume that no liquid wastewater flow from the onsite wastewater treatment plant is sent to a landfill and set  $q_-OW_-LF_{i,p,l,t}=0$ . However, there is solid waste flow. The solid wastes come from drilling rocks, wastewater sediments, and the chemicals added during the onsite wastewater pretreatment and treatment. This will be discussed further in the solid waste generation section. We assume that solid waste generation is a function of wastewater quantity and concentration and that no wastewater is sent to a landfill.

For onsite wastewater treatment technology i on well pad p,  $OW_{i,p}$ , the inflow of the onsite wastewater treatment plant should be less than or equal to the wastewater treatment capacity:

$$q_{S1} = OW_{i,p,t} \le cap_{OW_{i,p}}, \forall i, p, t$$

$$\tag{5}$$

We further assume no liquid loss and no wastewater sent to a landfill. Hence we have the following water balance constraint at the onsite wastewater treatment facility:

$$q_{S1}OW_{i,p,t} = q_{OW}S2_{i,p,t} + \sum_{l} q_{OW}LF_{i,p,l,t}, \forall i, p,t$$
 (6)

$$q_{-}OW_{-}LF_{i,p,l,t} = 0, \qquad \forall i, p, l, t \tag{7}$$

For S2 storage at pad p in time period t, it should be equal to the storage at the end of previous time period, t-1, plus effluent from onsite wastewater treatment minus reclaimed water sent to other wells in pad p for hydraulic fracturing, minus wastewater sent to deep well d for injection, minus wastewater sent to storage for selling in the reclaimed water market and minus wastewater sent to surface water discharge.

$$S2_{p,t} = S2_{p,t-1} + \sum_{i} q_{-}OW_{-}S2_{i,p,t} - \sum_{w} q_{-}S2_{-}W_{w,p,t}$$

$$-\sum_{t} q_{-}S2_{-}D_{p,d,t} - q_{-}S2_{-}S4_{p,c,t} - q_{-}S2_{-}R_{p,t}$$
(8)

Furthermore, S2 storage at pad p at time period t should be less than or equal to S2 design capacity:

$$S2_{p,t} \le cap \_S2_p , \forall p,t$$
 (9)

The influent storage of centralized wastewater treatment facility c at time period t,  $S3_{c,t}$ , equals the storage at the end of previous time period t-I, plus inflow from storage  $SI_{p,t}$  of all pads, minus wastewater sent to individual centralized wastewater treatment technology i:

$$S3_{c,t} = S3_{c,t-1} + \sum_{p} q_{-}S1_{-}S3_{p,c,t} - \sum_{i} q_{-}S3_{-}CW_{i,c,t} , \forall c,t$$
 (10)

$$S3_{c,0} = 0$$
 (11)

The design capacity constraint of the influent storage  $S3_{c,t}$  can be expressed as

$$S3_{c,t} \le cap \_S3_c , \forall c,t$$
 (12)

The design capacity constraint for individual centralized wastewater treatment technology i can be expressed as

$$q_{S3}CW_{i,c,t} \le cap_{CW_{i,c}}, \forall i, c, t \tag{13}$$

The outflow from CWT facilities, assuming there is no water loss, is split into two streams. One stream is stored in *S4* for sale in the reclaimed water market. The other stream is released into the river for discharge. This occurs if there is no demand and the storage is full.

$$q_{S3}CW_{i,c,t} = q_{CW}S4_{i,c,t} + q_{CW}R_{i,c,t}, \forall i,c,t$$
 (14)

The effluent storage S4 at centralized wastewater treatment plant c and at time period t equals the storage at the previous time period plus inflow, minus outflows, which include water reused for hydraulic fracturing and for other beneficial uses, during this time period:

$$S4_{c,t} = S4_{c,t-1} + \sum_{i} q_{-}CW_{-}S4_{i,c,t} - \sum_{p} \sum_{w} q_{-}S4_{-}W_{c,w,p,t} - q_{-}S4_{-}OD_{c,t} , \forall c,t$$
 (15)  

$$S4_{c,0} = 0$$
 (16)

The design capacity constraint of S4 can be expressed as

$$S4_{c,t} \le cap \_S4_c , \forall c,t \tag{17}$$

### **4.4.3** Chemical Balance Constraints

Water quality requirements of fracking fluid and wastewater discharge standards are based on chemical concentrations. To estimate chemical concentration, it is necessary to keep track of the chemical mass balance in addition to the water balance in the system. In this section, we conduct chemical mass balance using total dissolved solids (TDS) as an example.<sup>13</sup> Future work will include at least one other pollutant.

We assume that the TDS concentration from all freshwater sources is 0, and hence  $c_F W_{w,p,t} = 0$ , for all p, w, and t.

The TDS concentration in the water for fracking fluid preparation has to be lower than a specified limit:

<sup>&</sup>lt;sup>13</sup> TDS is a major concern for hydraulic fracturing using slick water hydraulic fracturing technology.

$$(\sum_{f} c - F - W_{f,w,p,t} \times q - F - W_{f,w,p,t}) + c - S2 - W_{w,p,t} \times q - S2 - W_{w,p,t} + c - S4 - W_{c,w,p,t} \times q - S4 - W_{w,p,t}$$

$$/(\sum_{f} q - F - W_{f,w,p,t}) + q - S2 - W_{w,p,t} + q - S4 - W_{c,w,p,t} \le \text{TDS\_limit}, \quad \forall c, w, p, t$$
(18)

We assume that we have complete knowledge about the TDS concentration profile in the flowback and produced wastewater stream over time for all the wells at all pads, and they are given by the model user or well developer:

$$c_{W_s} SI_{w,p,t} = conc_{W} WG_{w,p,t} , \forall w, p, t$$

$$(19)$$

Storage *S1* is a complete mixing reactor, and the concentration in the storage is the same as all the effluents from the storage. Thus, the current pollutant mass in the storage is equal to previous pollutant mass plus pollutant mass flow into the storage during this time period minus mass sent to CWTs, onsite wastewater treatment facilities, and deep injection wells:

$$c_{-}S1_{p,t} \times S1_{p,t} = c_{-}S1_{p,t-1} \times S1_{p,t-1} + (\sum_{w} c_{-}W_{-}S1_{w,p,t} \times q_{-}W_{-}S1_{w,p,t}) - \forall p,t \ (20)$$

$$c_{-}S1_{p,t} \times q_{-}S1_{-}S3_{p,c,t} - c_{-}S1_{p,t} \times \sum_{i} q_{-}S1_{-}OW_{i,p,t} - c_{-}S1_{p,t} \times \sum_{d} q_{-}S1_{-}D_{p,d,t}$$

If we rearrange the above equation, we have

$$c_{-}S1_{p,t} \times (S1_{p,t} + q_{-}S1_{-}S3_{p,c,t} + \sum_{i} q_{-}S1_{-}OW_{i,p,t} + q_{-}S1_{-}D_{p,d,t}) =$$

$$\forall p,t \ (21)$$

$$c_{-}S1_{p,t-1} \times S1_{p,t-1} + (\sum_{w} c_{-}W_{-}S1_{w,p,t} \times q_{-}W_{-}S1_{w,p,t})$$

Hence, the TDS concentration in the storage SI of pad p at the end of the time period t can be derived as

$$c_{-}S1_{p,t} = \frac{c_{-}S1_{p,t-1} \times S1_{p,t-1} + (\sum_{w} c_{-}W_{-}S1_{w,p,t} \times q_{-}W_{-}S1_{w,p,t})}{(S1_{p,t} + q_{-}S1_{-}S3_{p,c,t} + \sum_{i} q_{-}S1_{-}OW_{i,p,t} + \sum_{d} q_{-}S1_{-}D_{p,d,t})} \quad \forall p,t (22)$$

The concentrations in the three outflows of storage S1 would be all the same and shown as

$$c_{-}S1_{p,t} = c_{-}S1_{-}S3_{p,c,t}$$

$$c_{-}S1_{p,t} = c_{-}S1_{-}D_{p,d,t} \qquad \forall i, p, d, t$$
(23)

$$c \, \_\, S1_{p,t} = c \, \_\, S1 \, \_\, OW_{i,p,t}$$

To determine the concentration of the effluent of onsite wastewater treatment, we assume onsite wastewater treatment could include three treatment technologies: Technology 1 (primary), Technology 2 (primary + secondary), and Technology 3 (primary + secondary + tertiary). The TDS removal rate of an individual technology is given and can be represented using a removal coefficient,  $r_{-}OW_{i,p}$ . The effluent concentration can be expressed as

$$c_{OW\_S2_{i,p,t}} = (1 - r_{OW_{i,p}}) \times c_{S1\_OW_{i,p,t}} \quad \forall i, p, t$$
 (24)

For simplicity, we assume the water loss rate of individual technology is very small and can be ignored and that wastewater in storage S2 is completely mixed. Thus, the concentration at storage S2 and its outflow stream can be expressed as

$$c_{-}S2_{p,t} = \frac{c_{-}S2_{p,t-1} \times S2_{p,t-1} + \sum_{i} c_{-}OW_{-}S2_{i,p,t} \times q_{-}OW_{-}S2_{i,p,t}}{S2_{p,t-1} + \sum_{i} q_{-}OW_{-}S2_{i,p,t}} \quad \forall p,t$$
 (25)

The decision variables are the amount of water allocated to the individual treatment technology, I,  $q_{-}OW_{-}S2_{i,p,t}$  at well pad p and time t. The concentration of reclaimed wastewater reused in fracking fluid is equal to concentration of the outflow from storage S2:

$$c \_S2 \_W_{w,p,t} = c \_S2_{p,t} \qquad \forall w, p, t$$
 (26)

The storage  $S3_c$  denotes the influent storage capacity at a CWT facility, c. The pollutant concentration at any time in storage  $S3_{c,t}$  and its outflow stream can be expressed as

$$c\_S3_{c,t} = \frac{c\_S3_{c,t-1} \times S3_{c,t-1} + \sum_{p} c\_S1\_S3_{p,c,t} \times q\_S1\_S3_{p,c,t} - \sum_{i} c\_S3\_CW_{i,c,t} \times q\_S3\_CW_{i,c,t}}{\sum_{i} q\_S3\_CW_{i,c,t}} \, \forall c,t \, \, (27)$$

The pollutant concentration of the influent of the CWT can be denoted as

$$c_S3_CW_{c,t} = c_S3_{c,t} \qquad \forall c,t$$
 (28)

The pollutant concentrations in the CWT effluent from technology *i*, sent to surface water discharge and storage *S4* for reclaimed water market is equal to the CWT influent concentration times one minus pollutant removal rate

$$c \ CW \ R_{i,c,t} = c \ S3 \ CW_{i,c,t} \times (1 - r \ CW_{i,c}) \quad \forall c,t$$
 (29)

$$c CW S4_{i,c,t} = c S3 CW_{i,c,t} \times (1 - r CW_{i,c}) \quad \forall c,t$$
 (30)

### **4.4.4 Environmental Considerations**

Siting of Centralized Wastewater Treatment (CWT) Facilities

It is expensive for well operators to transport wastewater from (distributed) wells to an offsite CWT. A CWT planner may consider a system of multiple regional CWTs instead of a single big CWT to lower well operators' transportation costs and provide incentives for well operators to ship their wastewater to offsite CWT. Such systems could also reduce environmental externalities.

A CWT planner may consider building a limited number of CWT facilities. A planner who wants to build only *N* CWTs could accomplish this through the following constraints:

$$q \_S1\_S3_{p,c,t} \le M \times y_c \qquad \forall p,c,t ;$$
 (31); and

$$\sum_{c} y_{c} = N \tag{32}$$

Where, M is a large positive number,  $y_c$  is a binary opening variable, and N is the number of CWT plants that an operator would like to open. When there is a shipment and  $q_S1_S3_{p,c,t}$  that is greater than zero,  $q_S1_S3_{p,c,t}/M$  is small positive number. Since  $y_c$  is a binary (0,1) variable, it means that  $y_c = 1$ , and hence CWT, c, is built.

#### Solid Waste Generation

The amount of solid waste generated depends on the concentration and quantity of wastewater inflow and the treatment technology. The solid waste production function may be derived empirically. Future work will involve empirical analysis to calibrate the solid waste generation function f using real-world data. The model currently assumes that the amount of solid waste generated equals a technology-specific factor times the mass of pollutant removed during the treatment process. The solid waste generated from onsite wastewater treatment technology i in pad p is then sent to various landfills, LF.

$$s_{-}OW_{i,p,t} = f(c_{-}S1_{-}OW_{i,p,t}, q_{-}S1_{-}OW_{i,p,t}) = sw_{-}factor_{i} \times r_{-}OW_{i,p} \times c_{-}S1_{-}OW_{i,p,t} \times q_{-}S1_{-}OW_{i,p,t} \qquad \forall i, p, t$$
 (33)

$$s \_OW_{i,p,t} = \sum_{l} s \_OW \_LF_{i,p,l,t}, \qquad \forall i, p, t$$
(34)

The same process for solid waste generation applies to solid waste generation from CWT and can be expressed using the following two equations:

$$s_{-}CW_{i,c,t} = f(c_{-}S3_{-}CW_{i,c,t}, q_{-}S3_{-}CW_{i,c,t}) =$$

$$sw_{-}factor_{i} \times r_{-}CW_{i,c} \times c_{-}S3_{-}CW_{i,c,t} \times q_{-}S3_{-}CW_{i,c,t} \qquad \forall i, c, t \qquad (35)$$

$$s \_CW_{i,c,t} = \sum_{t} s \_CW \_LF_{i,c,l,t}, \qquad \forall i, c, t$$
(36)

### Landfill Capacity Constraint

For every landfill, *l*, the accepted solid waste at any time period should be smaller than the landfill capacity.

$$\sum_{i} \sum_{c} s CW LF_{i,c,l,t} + \sum_{i} \sum_{p} s OW LF_{i,p,l,t} \le cap LF_{l}$$
  $\forall l,t$  (37)

### Deep Well Injection Capacity Constraint

The amount of water from all well pads and CWT plants disposed of via deep well injection should be less than the capacity for every injection well, D:

$$\sum_{p} q_{-}S1_{-}D_{p,d,t} + \sum_{c} q_{-}S4_{-}D_{c,d,t} \le cap_{-}D_{d} , \quad \forall d,t$$
 (38)

#### Seismicity Risk (SR)

Seismicity risk associated with a specific deep injection well, d, in time period t can be expressed as a function of total injection within that time period. Note that we assume seismicity activity (magnitude and frequency) is correlated with incremental wastewater injection but not the historical cumulative injection. A general seismicity risk function  $f_s$  can be expressed as

$$f_{s}(\sum_{p} q_{-}S1_{-}D_{p,d,t} + \sum_{c} q_{-}S4_{-}D_{c,d,t} \mid \theta)$$
(39)

Where,  $\theta$  is a set of the functional parameters. The exact functional form will have to be determined through empirical data analysis.<sup>14</sup>

Assuming that increases in seismicity risk due to additional wells are the same regardless of the number of existing wells (density), then every well can be treated independently. Seismic risk for a

<sup>&</sup>lt;sup>14</sup> To identify the factors which cause a seismic event is an ongoing popular research topic (National Academies of Sciences 2016).

given region and time will be a linear summation of seismicity risk of individual wells, and total seismicity risk can then be expressed as the summation over all the injections over time and over all wells.

$$SR = \sum_{d} \sum_{t} f_{s} \left( \sum_{p} q_{-} S1_{-} D_{p,d,t} + \sum_{c} q_{-} S4_{-} D_{c,d,t} \mid \theta \right)$$
 (40)

Population Exposure to Traffic Accident and Spills (PETAS)

In this section, we measure the population exposure risk to tank truck accident and spills using a method similar to Ak and Bozkaya (2008). For every transportation link, the measurement of population exposure risk is found by multiplying five elements and can be expressed in the following way:

Population exposure risk = truck accident rate (in number of accidents per vehicle-mile) x

the length of the link x

the probability of release given that an accident has happened x

the number of people in a danger circle along a unit link x

wastewater shipment quantity

For example, consider link  $S1\_D_{p,d}$  that ships wastewater from storage S1 at well pad p to deep well d,  $a\_S1\_D_{p,d}$  is the tank truck accident rate;  $q\_S1\_D_{p,d,t}$  is the quantity of wastewater shipped on the link during time period t;  $d\_S1\_D_{p,d}$  is the length of the link;  $prob\_S1\_D_{p,d}$  is the probability of release given an accident; and  $p\_S1\_D_{p,d}$  is the population exposed to risk around the truck's danger circle, which is defined as the area of the danger circle times the population density around the link. We minimize population exposure in the objective function. This way, the model will determine the trade-off between the amount of wastewater shipped and population exposure. An operator can choose to ship a small quantity through a high population link or ship a large quantity through a low population link.

The population exposure to traffic accidents and spills for all the shipment links can be expressed as follows:

$$PETAS =$$

$$(\sum_{f} \sum_{w} \sum_{p} \sum_{t} a \_F \_W_{f,p} \times d \_F \_W_{f,p} \times prob \_F \_W_{f,p} \times p \_F \_W_{f,p} \times q \_F \_W_{f,w,p,t}) + C_{f} \sum_{w} \sum_{p} \sum_{t} a \_F \_W_{f,p} \times d \_F \_W_{f,p} \times prob \_F \_W_{f,p} \times p \_F \_W_{f,p} \times q \_F \_W_{f,w,p,t}) + C_{f} \sum_{w} \sum_{p} \sum_{t} a \_F \_W_{f,p} \times d \_F \_W_{f,p} \times prob \_F \_W_{f,p} \times p \_F \_W_{f,p} \times q \_F \_W_{f,p} \times$$

$$(\sum_{p} \sum_{d} \sum_{t} a\_S1\_D_{p,d} \times d\_S1\_D_{p,d} \times prob\_S1\_D_{p,d} \times p\_S1\_D_{p,d} \times q\_S1\_D_{p,d,t}) + \\$$

$$(\sum_{p}\sum_{c}\sum_{t}a_{-}S1_{-}S3_{p,c} \times d_{-}S1_{-}S3_{p,c} \times prob_{-}S1_{-}S3_{p,c} \times p_{-}S1_{-}S3_{p,c} \times q_{-}S1_{-}S3_{p,c}) + (\sum_{p}\sum_{t}\sum_{t}a_{-}CW_{-}R_{c} \times d_{-}CW_{-}R_{c} \times prob_{-}CW_{-}R_{c} \times p_{-}CW_{-}R_{c} \times q_{-}CW_{-}R_{i,c,t}) + (\sum_{p}\sum_{t}a_{-}S2_{-}R_{p} \times d_{-}S2_{-}R_{p} \times prob_{-}S2_{-}R_{p} \times p_{-}S2_{-}R_{p} \times q_{-}S2_{-}R_{p,t}) + (\sum_{p}\sum_{t}a_{-}S2_{-}S4_{p,c} \times d_{-}S2_{-}S4_{p,c} \times prob_{-}S2_{-}S4_{p,c} \times p_{-}S2_{-}S4_{p,c} \times q_{-}S2_{-}S4_{p,c,t}) + (\sum_{c}\sum_{t}a_{-}S4_{-}D_{c,d} \times d_{-}S4_{-}D_{c,d} \times prob_{-}S4_{-}D_{c,d} \times p_{-}S4_{-}D_{c,d} \times q_{-}S4_{-}D_{c,d,t}) + (\sum_{c}\sum_{t}a_{-}S4_{-}R_{c} \times d_{-}S4_{-}R_{c} \times prob_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c} \times q_{-}S4_{-}R_{c,t}) + (\sum_{c}\sum_{t}a_{-}S4_{-}R_{c} \times d_{-}S4_{-}R_{c} \times prob_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c,t}) + (\sum_{c}\sum_{t}a_{-}S4_{-}R_{c} \times d_{-}S4_{-}R_{c} \times prob_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c,t}) + (\sum_{c}\sum_{t}a_{-}S4_{-}R_{c} \times d_{-}S4_{-}R_{c} \times prob_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c,t}) + (\sum_{t}\sum_{t}a_{-}S4_{-}R_{c} \times d_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c}) + (\sum_{t}\sum_{t}a_{-}S4_{-}R_{c} \times p_{-}S4_{-}R_{c} \times p_{-}S4_$$

Surface Water Discharge (SWD)

The quality of surface water discharge from CWT facilities is constrained in the model. The CWT effluent concentration (influent concentration times one minus pollutant removal efficiency using treatment technology *i*) must be in compliance with effluent discharge standards.

$$c CW R_{i,c,t} = c S3 CW_{i,c,t} \times (1 - r CW_{i,c}) \le Discharge\_std$$
  $\forall i, c, t$  (42)

Currently, the model considers adherence to the effluent discharge standard only at the point of discharge. In the future, we plan to consider pollutant transport and pollutant loading in downstream water bodies by linking point-source discharges with a water quality model, such as the US Geological Survey SPARROW model.

#### Air Emissions (AE)

The model includes emissions from transportation. We include conventional air pollutants, such as  $NO_x$  and  $PM_{2.5}$ , and greenhouse gases, such as  $CO_2$ . For each transportation link in our system, the emissions of a specific air pollutant, j, are expressed as an emissions factor  $(EF_j)$  in grams per ton per mile, times the length of the link in miles and the quantity of the shipment. Currently, the model considers only transportation emissions of air pollutants. In the future, we could extend the model to include transportation impacts on local and regional ambient air quality and public health by linking air emissions estimation from this work with an ambient air quality model and human dose-response functions, such as those found in APEEP (Muller and Mendelsohn 2006).

$$\begin{split} Emissions_{j} &= \\ &(\sum_{f} \sum_{w} \sum_{p} \sum_{t} EF_{j} \times d - F - W_{f,p} \times q - F - W_{f,w,p,t}) + \\ &(\sum_{p} \sum_{d} \sum_{t} EF_{j} \times d - S1 - D_{p,d} \times q - S1 - D_{p,d,t}) + \\ &(\sum_{p} \sum_{c} \sum_{t} EF_{j} \times d - S1 - S3_{p,c} \times q - S1 - S3_{p,c,t}) + \\ &(\sum_{p} \sum_{c} \sum_{t} EF_{j} \times d - CW - R_{c} \times q - CW - R_{i,c,t}) + \\ &(\sum_{p} \sum_{t} EF_{j} \times d - S2 - R_{p} \times q - S2 - R_{p,t}) + \\ &(\sum_{p} \sum_{c} \sum_{t} EF_{j} \times d - S2 - S4_{p,c} \times q - S2 - S4_{p,c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - D_{c,d} \times q - S4 - D_{c,d,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} EF_{j} \times d - S4 - R_{c} \times q - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} EF_{j} \times d - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} EF_{j} \times d - S4 - R_{c,t}) + \\ &(\sum_{c} \sum_{t} EF_{j} \times d - EF_{j} \times d -$$

$$(\sum_{i} \sum_{p} \sum_{l} \sum_{t} EF_{j} \times d _{O}W _{L}F_{p,l} \times s _{O}W _{L}F_{i,p,l,t}) + (\sum_{i} \sum_{c} \sum_{l} \sum_{t} EF_{j} \times d _{C}W _{L}F_{c,l} \times s _{C}W _{L}F_{i,c,l,t})$$

$$(43)$$

### 4.4.5 Cost Functions

Costs considered include water acquisition, water shipment, onsite treatment facility capital and O&M costs, centralized wastewater treatment plant capital and O&M costs, solid waste transportation cost and tipping fee, onsite storage cost (impoundment capital cost or tank O&M cost), and deep well injection costs.

Water Acquisition Cost (WAC)

The water acquisition cost includes the freshwater price multiplied by the quantity of water purchased from freshwater sources and the reclaimed water price times the quantity of reclaimed water purchased from CWT facilities.

$$WAC = PFWater_t \times \left(\sum_{f} \sum_{w} \sum_{p} \sum_{t} q_{-}F_{-}W_{f,w,p,t}\right) + PRWater_t \times \left(\sum_{c} \sum_{w} \sum_{p} \sum_{t} q_{-}S4_{-}W_{c,w,p,t}\right)$$
(44)

Truck Transportation Cost (TTC)

The truck transportation cost includes the cost of operating tank trucks (in dollars per bbl-mile for water and wastewater or dollars per ton-mile for solid waste) times the water and wastewater shipment distance, and shipment quantity and truck unit cost (in dollars per ton-mile for solid waste) times the solid waste shipment distance and shipment quantity.

$$TTC = \\ (\sum_{f} \sum_{w} \sum_{p} \sum_{t} q_{-}F_{-}W_{f,w,p,t} \times d_{-}F_{-}W_{f,p}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}S1_{-}D_{p,d,t} \times d_{-}S1_{-}D_{p,d}) \times tanktruckcost + \\ (\sum_{p} \sum_{c} \sum_{t} q_{-}S1_{-}S3_{p,c,t} \times d_{-}S1_{-}S3_{p,c}) \times tanktruckcost + \\ (\sum_{p} \sum_{c} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times tanktruckcost + \\ (\sum_{p} \sum_{d} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}CW_{-}$$

$$(\sum_{p}\sum_{t}q_{-}S2_{-}R_{p,t}\times d_{-}S2_{-}R_{p})\times tanktruckcost +$$

$$(\sum_{p}\sum_{c}\sum_{t}q_{-}S2_{-}S4_{p,c,t}\times d_{-}S2_{-}S4_{p,c})\times tanktruckcost +$$

$$(\sum_{c}\sum_{d}\sum_{t}q_{-}S4_{-}D_{c,d,t}\times d_{-}S4_{-}D_{c,d})\times tanktruckcost +$$

$$(\sum_{c}\sum_{t}q_{-}S4_{-}R_{c,t}\times d_{-}S4_{-}R_{c})\times tanktruckcost +$$

$$(\sum_{c}\sum_{w}\sum_{p}\sum_{t}q_{-}S4_{-}W_{c,w,p,t}\times d_{-}S4_{-}W_{c,p})\times tanktruckcost +$$

$$(\sum_{c}\sum_{t}q_{-}S4_{-}OD_{c,t}\times d_{-}S4_{-}OD_{c})\times tanktruckcost +$$

$$(\sum_{t}\sum_{p}\sum_{t}\sum_{s}S_{-}OW_{-}LF_{i,p,l,t}\times d_{-}OW_{-}LF_{p,l})\times truckcost +$$

$$(\sum_{t}\sum_{s}\sum_{t}\sum_{s}S_{-}CW_{-}LF_{i,c,l,t}\times d_{-}CW_{-}LF_{c,l})\times truckcost +$$

$$(45)$$

## Pipe Transportation Cost (PTC)

The pipeline transportation cost is the pipeline unit cost (in dollars per bbl-mile for water and wastewater) times shipment distance and shipment quantity for fresh water and wastewater.

$$PTC = \\ (\sum_{f} \sum_{w} \sum_{p} \sum_{t} q_{-}F_{-}W_{f,w,p,t} \times d_{-}F_{-}W_{f,p}) \times pipecost + \\ (\sum_{p} \sum_{d} \sum_{t} q_{-}S1_{-}D_{p,d,t} \times d_{-}S1_{-}D_{p,d}) \times pipecost + \\ (\sum_{p} \sum_{c} \sum_{t} q_{-}S1_{-}S3_{p,c,t} \times d_{-}S1_{-}S3_{p,c}) \times pipecost + \\ (\sum_{i} \sum_{c} \sum_{t} q_{-}CW_{-}R_{i,c,t} \times d_{-}CW_{-}R_{c}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{p} \sum_{t} q_{-}S2_{-}R_{p,t} \times d_{-}S2_{-}R_{p}) \times pipecost + \\ (\sum_{t} q_{-}S2_{-}R_{p$$

$$(\sum_{p} \sum_{c} \sum_{t} q_{-}S2_{-}S4_{p,c,t} \times d_{-}S2_{-}S4_{p,c}) \times pipecost +$$

$$(\sum_{c} \sum_{d} \sum_{t} q_{-}S4_{-}D_{c,d,t} \times d_{-}S4_{-}D_{c,d}) \times pipecost +$$

$$(\sum_{c} \sum_{t} q_{-}S4_{-}R_{c,t} \times d_{-}S4_{-}R_{c}) \times pipecost +$$

$$(\sum_{c} \sum_{w} \sum_{p} \sum_{t} q_{-}S4_{-}W_{c,w,p,t} \times d_{-}S4_{-}W_{c,p}) \times pipecost +$$

$$(\sum_{c} \sum_{t} q_{-}S4_{-}OD_{c,t} \times d_{-}S4_{-}OD_{c}) \times pipecost +$$

$$(\sum_{i} \sum_{p} \sum_{t} \sum_{t} s_{-}OW_{-}LF_{i,p,l,t} \times d_{-}OW_{-}LF_{p,l}) \times pipecost +$$

$$(\sum_{i} \sum_{c} \sum_{t} \sum_{t} s_{-}CW_{-}LF_{i,c,l,t} \times d_{-}CW_{-}LF_{c,l}) \times pipecost +$$

$$(46)$$

## Onsite Treatment Capital Cost (OWCC)

Onsite treatment capital costs include costs for the onsite wastewater treatment technologies, onsite wastewater storage, and onsite reclaimed water storage. We assume a linear function. In future work, we plan to generalize the linear function to nonlinear functions in order to consider economies of scale or diseconomies of scale.

$$OWCC =$$

$$\sum_{i} \sum_{p} capcost _{-}OW_{i} \times cap _{-}OW_{i,p} + \sum_{p} capcost _{-}S1 \times cap _{-}S1_{p} + \sum_{p} capcost _{-}S2 \times cap _{-}S2_{p}$$

$$(47)$$

Operator O&M Costs for Onsite Treatment and Waste Disposal (OWOM)

The O&M costs for well operators include costs for onsite wastewater treatment and Class II well injections and solid waste landfill tipping fees:

$$OWOM =$$

$$\sum_{i} omcost \_OW_{i} \times (\sum_{p} \sum_{t} q\_S1\_OW_{i,p,t}) + \sum_{d} omcost \_D_{d} \times (\sum_{p} \sum_{t} q\_S1\_D_{p,d,t}) +$$

$$\sum_{t} omcost \_LF_{l} \times \sum_{i} \sum_{s} \sum_{t} s\_OW\_LF_{i,p,l,t}$$

$$(48)$$

CWT Capital Cost (CWCC)

CWT capital costs include costs for the centralized wastewater treatment technologies, influent storage, and reclaimed water storage. We assume a linear function. For future work, we plan to generalize the linear function to nonlinear functions in order to consider economies of scale or diseconomies of scale.

CWCC =

$$\sum_{i} \sum_{c} capcost \ CW_{i} \times cap \ CW_{i,p} + \sum_{c} capcost \ S3 \times cap \ S3_{c} + \sum_{c} capcost \ S4 \times cap \ S4_{c}$$
(49)

CWT O&M Cost (CWOM)

CWT O&M costs include costs for CWT, Class II well injections, and solid waste landfill tipping fees:

CWOM =

$$\sum_{i} omcost \ \_CW_{i} \times (\sum_{c} \sum_{t} q \_S3 \_CW_{i,c,t}) + \sum_{d} omcost \ \_D_{d} \times (\sum_{p} \sum_{t} q \_S1 \_D_{p,d,t}) +$$

$$\sum_{l} omcost \ \_LF_{l} \times \sum_{i} \sum_{c} \sum_{t} s \_CW \_LF_{i,c,l,t}$$

$$(50)$$

Reclaimed Water Market Revenue (RWMR)

The reclaimed water market revenue is the revenue that CWT facility operators receive by selling reclaimed water to well operators for hydraulic fracturing and water sold to others who demand reclaimed water for other beneficial uses. Revenue equals the quantity of water at a particular treatment level multiplied by the price of water with that level of water quality. We assume prices in the reclaimed water are determined exogenously and reflect the quality of the treated water.

$$RWMR = (\sum_{c} \sum_{t} q_{-}S4_{-}OD_{c,t} + \sum_{c} \sum_{w} \sum_{p} \sum_{t} q_{-}S4_{-}W_{c,w,p,t}) \times PRWater_{t}$$
 (51)

### 4.4.6 Revenue Sources

Resource Recovery Revenue (RRR)

We assume that some materials—for example, gypsum and iodine—can be recovered during treatment at CWT facilities. The resource recovery revenue equals the wastewater treated times a material recovery factor times the price of the recovered material.

$$RRR = \sum_{t} \left( \left( \sum_{c} \sum_{i} q_{-}S3_{-}CW_{i,c,t} \right) \times MRF \right) \times PRMR_{t}$$
 (52)

### **4.4.7 Objective Functions**

For well operators, the objective is to minimize water acquisition costs (WAC), truck transportation costs (TTC), pipeline transportation costs (PTC), onsite treatment capital costs (OWCS), and onsite treatment and waste disposal costs (OWOM). The objective function for well operators can be expressed as

$$OBJ1 = Minimize WAC + TTC + PTC + OWCC + OWOM$$

For CWT planners, the objective is to minimize CWT capital costs (CWCS) and CWT O&M costs (CWOM) and maximize revenue from the reclaimed water market, including both reclaimed water market revenue (RWMR) and resource recovery revenue (RRR). The objective function for CWT planners can be expressed as

$$OBJ2 = Minimize CWCC + CWOM - RWMR - RRR$$

For regulators, the objective is to minimize population exposure to traffic accidents and spills (PETAS), seismicity risk (SR), and air emissions (AE) and keep effluent from CWT facilities in compliance with surface water discharge standards (SWD). The objective function for regulators can be expressed as

$$OBJ3 = Minimize PETAS + SR + AE$$

The objective for the social planner is to combine the above three objective functions, subject to the wastewater discharge standard. The objective function for the social planner can expressed as

$$OBJ4 = Minimize OBJ1 + OBJ2 + OBJ3$$

Subject to: SWD

### 5. Model Solution and Data Issues

We have completed the development of a decisionmaking model for shale gas water and wastewater management. Although the model itself is generic, our next step is to calibrate the model to a specific region and conduct a case study, which will involve two challenges.

The first challenge is incorporating water pollutant concentration constraints. Our model specifically considers the relationship between the composition of wastewater, particularly with respect to the input water quality requirements for different treatment technologies, and the quality of effluent from CWT discharged to surface waterbodies for each of the water management options. To consider concentration constraints in our modeling system, we need to track the water and chemical

mass balance for the entire system. This makes our mathematical model formulation extremely nonlinear and nonseparable, and thus difficult to solve. Therefore, we will need to make simplifying assumptions and/or develop a tailored simulation-optimization algorithm for solving the model.

And second, collecting reliable data (in terms of the quality and quantity) is difficult. Some data are available from the literature, but some data are very uncertain, especially for the following three categories:

- Wastewater generation and wastewater concentration profiles. These data are highly variable
  and depend on the geological and operational conditions as well as chemical additives used in
  hydraulic fracturing fluid preparations. However, data are available for specific wells.
- Performance and economic data for tertiary treatment technologies. Treatment performance
  and costs are highly uncertain. Many of the treatment technologies require in-field tests, not
  just lab studies. It is important to test the technologies as part of an integrated system, not just a
  single component.
- Parameters for quantifying environmental externalities. Although we consider several
  transportation and seismic environmental externalities, we were not able to include in the
  model many other externalities—such as transportation accident and spill rates, seismicity risk,
  and solid waste production functions—because the risk exposure pathways are not fully
  understood at this moment.

In the following table, we list input data needed for the model. Input data include physical parameters or noneconomic inputs (e.g., water demand profiles, wastewater pollutant, pollutant removal efficiency of different treatment options, well capacity, relevant distances, and population exposure to risks), as well as economic inputs (e.g., transportation costs, capital costs, O&M costs, and disposal fees). In the third column, we provide possible sources of data for model calibration and a case study.

Noneconomic inputs Definition Data source Water demand profile at well w, pad p and time period t,  $WD_{w,p,t}$ Well operators gal/week TDS\_limit TDS concentration limit in the water preparing for Well operators  $WWG_{w,p,t}$ Flowback and produced (FP) wastewater generation Well operators profile from well w, pad p and time period t, gal/week  $conc_WWG_{w,p,t}$ Pollutant (TDS) concentration profile in the FP Well operators wastewater stream, ppm

**Table 3. Model Inputs** 

$r\_OW_{i,p}$	Pollutant removal efficiency at the onsite wastewater	Wastewater treatment experts
	treatment technology $i$ , at pad $p$ , %	
$r\_CW_{i,c}$	Pollutant removal efficiency at the CWT plant, c, using treatment technology i, %	Wastewater treatment experts
$cap\_D_d$	Injection/disposal capacity at deep well d, gal/week	Injection well operators
cap_LF <sub>l</sub>	Solid waste disposal capacity at landfill site <i>l</i> , tons/week	Landfill operators
$d_F_W_{f,p}$	Distance between fresh water source f and well w in pad	GIS analysis
	p, mile	·
$d\_S1\_D_{p,d}$	Distance between $SI$ in pad p and deep well $d$ , mile	GIS analysis
$d\_S1\_S3_{p,c}$	Distance between S2 in pad p and S3, mile	GIS analysis
$d\_S2\_D_{p,d}$	Distance between $S2$ in pad $p$ and deep well $d$ , mile	GIS analysis
$d_{CW}R_{c}$	Distance between CWT and location for surface water discharge, mile	GIS analysis
d_S2_R <sub>p</sub>	Distance between S2 in pad p and location for surface water discharge, mile	GIS analysis
$d_S2_S4_{p,c}$	Distance between S2 in pad p and S4, mile	GIS analysis
$d\_S4\_D_{c,d}$	Distance between S4 and deep well d, mile	GIS analysis
$d_S4R_c$	Distance between S4 and location for surface water	GIS analysis
	discharge, mile	·
$d_S4_W_{c,p}$	Distance between $S4$ and well w in pad $p$ , mile	GIS analysis
$d_S4_OD_c$	Distance between S4 and location for other demand of	GIS analysis
	reclaimed water, mile	
$d\_OW\_LF_{p,l}$	Distance between onsite wastewater treatment at pad <i>p</i>	GIS analysis
	and landfill site <i>l</i> , mile	
$d_{CW}LF_{c,l}$	Distance between CWT and landfill site <i>l</i> , mile	GIS analysis
$p_F_W_{f,p}$	Population exposure between fresh water source $f$ and well w in pad $p$ , mile	Census Bureau and GIS analysis
$p\_S1\_D_{p,d}$	Population exposure between $SI$ in pad $p$ and deep well $d$ , mile	Census Bureau and GIS analysis
<i>p_S1_S3<sub>p,c</sub></i>	Population exposure between S2 in pad p and S3, mile	Census Bureau and GIS analysis
p_S2_D <sub>p,d</sub>	Population exposure between S2in pad p and deep well d, mile	Census Bureau and GIS analysis
p_CW_R <sub>c</sub>	Population exposure between CWT and location for surface water discharge, mile	Census Bureau and GIS analysis
p_S2_R <sub>p</sub>	Population exposure between S2 in pad p and location for surface water discharge, mile	Census Bureau and GIS analysis
p_S2_S4 <sub>p,c</sub>	Population exposure between S2 in pad p and S4, mile	Census Bureau and GIS analysis
$p\_S4\_D_{c,d}$	Population exposure between S4 and deep well d, mile	Census Bureau and GIS analysis
p_S4_R <sub>c</sub>	Population exposure between <i>S4</i> and location for surface water discharge, mile	Census Bureau and GIS analysis
p_S4_W <sub>c,p</sub>	Population exposure between $S4$ and well w in pad $p$ , mile	Census Bureau and GIS analysis
p_S4_ODc	Population exposure between <i>S4</i> and location for other demand of reclaimed water, mile	Census Bureau and GIS analysis
$p\_OW\_LF_{p,l}$	Population exposure between onsite wastewater treatment at pad $p$ and landfill site $l$ , mile	Census Bureau and GIS analysis
p_CW_LF <sub>c,l</sub>	Population exposure between CWT and landfill site <i>l</i> , mile	Census Bureau and GIS analysis
$p\_F\_W_{f,p}$	Population exposure between fresh water source f and well w in pad <i>p</i> , mile	Census Bureau and GIS analysis

Economic inputs		
tanktruckcost	Tank truck transportation cost, \$/gal-mile	American Transportation Research Institute
pipecost	Pipe water transportation cost, \$/gal-mile	Well operators
truckcost	Truck transportation cost, \$/ton/mile, for shipping solid waste or hazardous materials	American Transportation Research Institute

capcost_OWi	Capital cost of onsite treatment technology <i>i</i> , \$/gal	Wastewater treatment experts or literature
capcost_CW <sub>i</sub>	Capital cost of centralized treatment technology <i>i</i> , \$/gal	Wastewater treatment experts or literature
capcost_S1	Capital cost of onsite storage <i>S1</i> , either impoundment or tank storage, \$/gal	Well operators or literature
capcost_S2	Capital cost of onsite storage S2, either impoundment or tank storage, \$/gal	Well operators or literature
capcost_S3	Capital cost of onsite storage <i>S3</i> , either impoundment or tank storage, \$/gal	Well operators or literature
capcost_S4	Capital cost of onsite storage <i>S4</i> , either impoundment or tank storage, \$/gal	Well operators or literature
omcost_OWi	O&M cost of onsite treatment technology <i>i</i> , as a function of flow, \$/gal	Wastewater treatment experts or literature
omcost_CWi	O&M cost of CWT treatment technology <i>i</i> , as a function of flow, \$/gal	Wastewater treatment experts or literature
omcost_tank	O&M cost of onsite tank storage, \$/gal	Wastewater treatment experts or literature
omcost_D	Deep well injection cost, \$/gal	Injection well operators
omcost_LF	Landfill tipping fee, \$/ton	Landfill operators

#### 6. Conclusion and Future Work

Although recent low oil and gas prices have slowed the rate of shale gas well drilling and wastewater generation, long-term forecasts for the natural gas industry suggest that shale gas development and associated wastewater quantities will grow. The water resources and wastewater management concerns necessitate an investigation using a systematic approach to ensure environmentally sustainable shale gas development. In this research, we adopt an integrated system analysis approach that looks at the entire life cycle of water in the hydraulic fracturing process.

Specifically, we conducted a literature review and developed a multi-objective mathematical programming model for shale gas water and wastewater management. This model is developed with four decisionmakers in mind: oil and gas well developers and operators, centralized wastewater treatment facility planners and operators, environmental and public health regulators, and social planners. For well developers and operators, the objective is to minimize water and wastewater management costs. For centralized wastewater treatment planners and operators, the objective is to minimize the capital and O&M costs of the wastewater treatment facility and maximize the revenue from selling reclaimed water and other recovered resources. For environmental regulators, the objective is to minimize environmental harms, such as pollutant loading in the surface water discharge, and ensure enforcement of other relevant laws. For social planners, the objective is to minimize social costs, which includes both private costs plus environmental costs (externalities).

This model could be used for simultaneously making decisions about water and wastewater management and infrastructure investments while considering environmental externalities. For example, the model could be used to optimize decisionmaking about wastewater treatment capital investment (onsite vs. an offsite centralized wastewater treatment facility), wastewater allocations to

various management options (onsite, centralized wastewater treatment, or deep well injection), and wastewater allocations to various treatment technologies and treatment levels (primary, secondary, and tertiary). It could also be used to evaluate environmental externalities resulting from allocation and investment decisions, or to site centralized wastewater treatment facilities to minimize transportation costs and environmental externalities, such as air emissions and population exposure to traffic accidents and spills. This model includes the reclaimed water and resource recovery market, which allows us to evaluate the economic incentives that would drive actors to participate in this market.

This research establishes a framework to analyze the optimal management of shale gas water and wastewater. Future work may include the following:

- including upstream system gas production revenue by generating a shale gas production function using well production data and including production revenue;
- considering the intermediate step of a centralized freshwater impoundment between freshwater withdraw and consumption;
- including road damage minimization in the objective function;
- calibrating the model with a case study and replacing current simple linear parameters for capital and O&M cost functions for various treatment technology and storage facility options;
- developing a solid waste production function based on technology-specific solid waste generation and water quality data;
- modeling reclaimed water of varying qualities for different beneficial uses (currently we treat reclaimed water as a uniform commodity and the market price as a given model input);
- including a more comprehensive reclaimed water component that includes demand and supply
  functions, to allow the model to determine reclaimed water price (currently we assume the
  prices of reclaimed water associated with specific water qualities are given but, we hope to
  collect reclaimed water market demand and supply data to endogenize the market prices of
  reclaimed water in our model);
- including more than one contaminant for optimization (currently we consider only total dissolved solids and track mass balance in the modeling system);
- refining the consideration of other resource recovery options for centralized wastewater treatment plants (currently we have only a simple representation of resource recovery);
- including other reclaimed water sources, such as reclaimed municipal wastewater, to supply water for well drilling and stimulation; and

• incorporating decisions about the expansion of existing centralized wastewater treatment facilities, in addition to building new facilities (currently we consider the investment in new facilities as wastewater management infrastructure).

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## **Appendix**

### Notes for Figure 1

This figure reflects the number of wells drilled between 2008 and 2015 and the amount of wastewater from this period. The number of wells drilled per year was obtained from the 2015 Oil and Gas Report and waste generation information based on the PADEP waste reports for January 2008 through December 2015. Data are only for unconventional wells. We calculated total wastewater volumes by summing quantities only for waste types identified as "brine," "fracking fluid waste," "fracking fluid," "fracking fluid waste," "fracking fluid waste (in barrels)," "produced fluid," and "produced fluid in barrels," by the year the wastewater was reported to PADEP. The number of spudded wells was calculated by summing the number of new wells per year, using the year provided in the spud date. We did not include wells that did not have an observation for the spud date variable. This value was missing for 637 (less than 6 percent) of the 9,635 wells. We limited our totals to the period from 2008 to 2015. A small number of wells had earlier spud dates, but they were omitted.

Table A1. Volumes of Fracking Wastewater in Pennsylvania, 2008–2015

Year	Total volume of wastewater	Number of drilled wells
2008	2,308,798	332
2009	8,026,636	818
2010	9,465,935	1,600
2011	35,300,000	1,957
2012	26,600,000	1,352
2013	33,000,000	1,215
2014	41,600,000	1,372
2015	38,000,000	785

#### Notes for Figure 2

This figure reflects information based on the PADEP waste reports for January 2008 through December 2015. The data are obtained when operators fill out mandated waste reports. They choose the disposal facility destination from a list of facilities that are registered with PADEP, and the disposal method field of the report is automatically populated with the permitted disposal method associated with that facility. Several other studies, such as Maloney and Yoxtheimer (2012), use this source and highlight some issues and inconsistencies with the data. We have not replicated the thorough cleaning and reclassification methods of these other studies. Data included in this chart are

only for unconventional wells and for waste types identified as "brine," "fracking fluid waste," or "produced fluid." The "other" category was created by combining the records where the disposal method was listed as "landfill," "residual waste processing facility," "residual waste transfer facility," "residual waste proc fac" (general permit), "other," and entries where the disposal method was listed as "identify method in comments." Some disposal method names were slightly modified to make them easier to read. Brine/industrial waste treatment plant was a disposal option only for 2008 and 2009.

Table A2. Disposal of Fracking Wastewater in Pennsylvania, 2008–2015

Year	Disposal method	Volume (bbls)	Percentage
2008	Brine/industrial waste treatment plant	718,982.50	31.19%
2008	Injection disposal well	5,882.50	0.26%
2008	Municipal sewage treatment plant	1,240,348.00	53.81%
2008	Other	304,268.80	13.20%
2008	Reuse other than road spreading	35,376.00	1.53%
2008	Road spreading	170.00	0.01%
2009	Brine/industrial waste treatment plant	5,146,336.00	64.19%
2009	Cwt facility for recycle	1,868.00	0.02%
2009	Injection disposal well	22,528.00	0.28%
2009	Municipal sewage treatment plant	1,381,437.00	17.23%
2009	Other	1,182,219.00	14.75%
2009	Reuse other than road spreading	283,263.00	3.53%
2009	Road spreading	75.00	0.00%
2010	Cwt facility for recycle	5,347,722.00	56.49%
2010	Injection disposal well	351,817.60	3.72%
2010	Municipal sewage treatment plant	146,584.40	1.55%
2010	Other	1,281,697.00	13.54%
2010	Reuse other than road spreading	2,251,232.00	23.78%
2010	Road spreading	596.00	0.01%
2010	Storage pending disposal or reuse	86,286.00	0.91%
2011	Cwt facility for recycle	4,912,447.00	27.81%
2011	Injection disposal well	2,183,863.00	12.36%
2011	Municipal sewage treatment plant	33,163.36	0.19%
2011	Other	51,325.38	0.29%
2011	Reuse other than road spreading	10,100,000.00	57.39%
2011	Storage pending disposal or reuse	345,483.10	1.96%
2012	Cwt facility for discharge	846.40	0.00%
2012	Cwt facility for recycle	2,988,964.00	11.24%
2012	Injection disposal well	3,564,206.00	13.40%

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2012	Other	153,543.00	0.58%
2012	Reuse other than road spreading	19,600,000.00	73.56%
2012	Road spreading	425.21	0.00%
2012	Storage pending disposal or reuse	320,929.00	1.21%
2013	Cwt facility for discharge	479,624.40	1.45%
2013	Cwt facility for recycle	1,699,001.00	5.15%
2013	Injection disposal well	3,242,215.00	9.83%
2013	Other	4,082,007.00	12.37%
2013	Reuse other than road spreading	23,300,000.00	70.77%
2013	Road spreading	105.00	0.00%
2013	Storage pending disposal or reuse	142,279.60	0.43%
2014	Cwt facility for discharge	1,183,022.00	2.85%
2014	Cwt facility for recycle	50,576.60	0.12%
2014	Injection disposal well	3,685,427.00	8.87%
2014	Other	9,746,719.00	23.45%
2014	Reuse other than road spreading	26,800,000.00	64.44%
2014	Road spreading	180.50	0.00%
2014	Storage pending disposal or reuse	110,127.30	0.27%
2015	Cwt facility for discharge	2,189,472.00	5.76%
2015	Cwt facility for recycle	1,744,584.00	4.59%
2015	Injection disposal well	2,649,631.00	6.97%
2015	Other	6,669,207.00	17.54%
2015	Reuse other than road spreading	24,700,000.00	65.02%
2015	Storage pending disposal or reuse	50,096.80	0.13%