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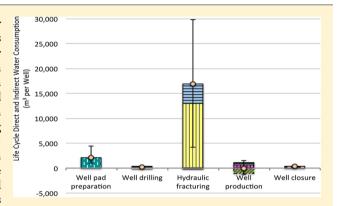
Life Cycle Water Consumption and Wastewater Generation Impacts of a Marcellus Shale Gas Well

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Supporting Information

ABSTRACT: This study estimates the life cycle water consumption and wastewater generation impacts of a Marcellus shale gas well from its construction to end of life. Direct water consumption at the well site was assessed by analysis of data from approximately 500 individual well completion reports collected in 2010 by the Pennsylvania Department of Conservation and Natural Resources. Indirect water consumption for supply chain production at each life cycle stage of the well was estimated using the economic input—output life cycle assessment (EIO-LCA) method. Life cycle direct and indirect water quality pollution impacts were assessed and compared using the tool for the reduction and assessment of chemical and other environmental impacts (TRACI). Wastewater treatment cost was proposed as an additional indicator for water quality pollution impacts from



shale gas well wastewater. Four water management scenarios for Marcellus shale well wastewater were assessed: current conditions in Pennsylvania; complete discharge; direct reuse and desalination; and complete desalination. The results show that under the current conditions, an average Marcellus shale gas well consumes 20 000 m³ (with a range from 6700 to 33 000 m³) of freshwater per well over its life cycle excluding final gas utilization, with 65% direct water consumption at the well site and 35% indirect water consumption across the supply chain production. If all flowback and produced water is released into the environment without treatment, direct wastewater from a Marcellus shale gas well is estimated to have 300–3000 kg N-eq eutrophication potential, 900–23 000 kg 2,4D-eq freshwater ecotoxicity potential, 0–370 kg benzene-eq carcinogenic potential, and 2800–71 000 MT toluene-eq noncarcinogenic potential. The potential toxicity of the chemicals in the wastewater from the well site exceeds those associated with supply chain production, except for carcinogenic effects. If all the Marcellus shale well wastewater is treated to surface discharge standards by desalination, \$59 000–270 000 per well would be required. The life cycle study results indicate that when gas end use is not considered hydraulic fracturing is the largest contributor to the life cycle water impacts of a Marcellus shale gas well.

INTRODUCTION

The Energy Information Administration (EIA) projected that shale gas will be expected to grow from 23% of total U.S. dry gas production in 2010 to 49% in 2035.1 The Marcellus shale formation in the Appalachian Basin, one of the most promising shale formations, is estimated to contain 780-1300 billion cubic meters (BCM) of technically recoverable natural gas. 1-4 As development of the Marcellus shale formation has increased, water management questions have arisen. Directional drilling and high-volume chemically amended hydraulic fracturing techniques have enabled economic shale gas extraction; however, these processes use large quantities of water.⁵⁻⁷ Also, wells produce large volumes of wastewater that requires treatment and disposal, including drilling wastewater, flowback, and produced water. Other wastewaters of smaller volumes include basic sediment, spent lubricant, and servicing fluid (representing 0.039% of the total waste fluids from Marcellus shale gas wells according to ref 8). Drilling wastewater is made

up of fluids, with a water base, used during the drilling process. Flowback water is the water that returns from the well during the flowback period, immediately after hydraulic fracturing and before gas production, approximately the first 10–14 days. Flowback water returns from the well at high flow rate but with relatively low concentrations of salinity, heavy metals (e.g., barium and strontium), and naturally occurring radioactive materials (NORM). Produced water is the water generated during gas production over the productive life of the well. Although the Marcellus shale is considered a relatively low water forming shale on a gas production basis (3.3–27 m³ water per million cubic meters (MCM) of gas 12), its development has increased the total oil- and gas-associated

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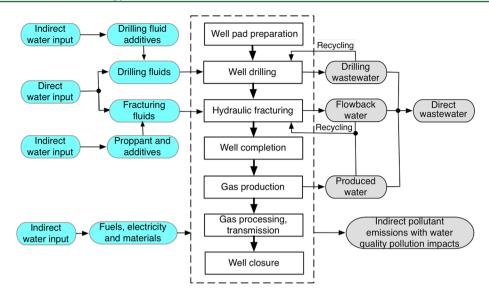


Figure 1. Life cycle processes of a Marcellus shale gas well. Rectangles bounded by the dotted lines in the center represent the major life cycle stages of a Marcellus shale well excluding gas utilization. Blue ovals on the left side show inputs to the well life cycle, and gray ovals on the right side show outputs from the well life cycle. Iindividual processes in the Marcellus shale well life cycle (e.g., drilling and fracturing) and direct water life cycle (e.g., transportation of water and treatment of wastewater) have supply chain production of fuels, electricity, and materials, which causes indirect water consumption and water quality pollution impacts.

wastewater generated in Pennsylvania by approximately 570% since 2004.¹³ Produced water returns at a lower rate but over the life of the well and with higher levels of salinity, ^{14,15} heavy metals, and NORM. ^{10,14,16} The chemicals in Marcellus shale wastewater may cause damage to the ecosystem and human health if not managed properly. ¹⁷

In addition to direct water use for drilling and fracturing operations at the well site, indirect water use for supply chain production of each well life cycle stage involves many water-intensive industrial sectors. The indirect supply chain water use and associated environmental impacts are generated across industrial activities and across watershed and state boundaries. A life cycle perspective offers a method for impact assessment accounting for direct and indirect water use for Marcellus shale gas wells. Only a few recent life cycle water studies on Marcellus shale gas have included indirect water use for supply chain production; 22-24 yet these studies have not incorporated the water quality pollution impacts caused by Marcellus shale well wastewater.

In order to inform sound decisions in water use and wastewater management for Marcellus shale gas development, life cycle water consumption and water quality pollution impacts must be considered. In the present work, a life cycle water impact assessment model for a Marcellus shale gas well, from its construction to its end of life, was developed. The impact assessment for each of the well life stages requires detailed information about the inputs to the system—water, materials, and energy—and the impacts of any outputs—wastewater, materials, and energy—on the environment. In the next section, the study analysis boundaries and functional unit are described, followed by details of data used and model assumptions. Results of the life cycle water impact assessment of the Marcellus shale gas well are presented along with the discussion of uncertainties.

ANALYSIS BOUNDARIES AND FUNCTIONAL UNIT

Functional Unit. We use a well as the assessment unit for Marcellus shale water impact in the Life Cycle Assessment

(LCA) structure (impacts/well), and we also report the impacts per megajoules of natural gas produced (impacts/MJ), which incorporates the uncertainty of gas production levels of Marcellus shale wells and is consistent with typical life cycle studies on production of energy fuels. 22,26

Life Cycle Stages Considered. The life cycle stages of a Marcellus shale gas well considered in our study are shown in Figure 1. Water impacts were assessed from Marcellus shale well pad preparation through delivery of shale gas to end user to well closure.²⁷ End use of shale gas, such as power generation, industrial use, residential heating, and transportation, are not included in the analysis boundaries; these uses also have water consumption and water quality pollution impacts ²² and are not considered in the present analysis.

For development of a Marcellus shale well, well site investigation occurs first, which has negligible water impacts and was excluded from analysis. After construction of the well pad and its access road, wells are drilled vertically and then horizontally with drilling equipment; drilling fluids are used, and drilling wastewater is generated in this stage. Well pads normally support multiple wells; we assume 6 (with a range of 1-16) wells per pad. ²⁸⁻³⁰ Hydraulic fracturing takes place after well drilling and uses a mixture of water, sand, and chemical amendments as hydraulic fracturing fluid. Fracturing waste fluid comes from the well as flowback water. Trucks are the predominant method to transport water to the well site, and truck transportation was assumed in the study, but sometimes pipes might also be used to transport water. Later, trucks are used to transport unrecycled wastewater and drilling cuttings from the well site to treatment or disposal locations. During well completion, wells are cased with steel and cemented to isolate downwell activities from the surrounding environment. Water use for steel casing and cement was not considered in the analysis; however, it is expected to represent less than 1% of the life cycle water use for shale gas well development. 22,24

After the well is completed, shale gas production starts and continues until the well is closed and capped at the end of its useful life. Produced water is generated with natural gas

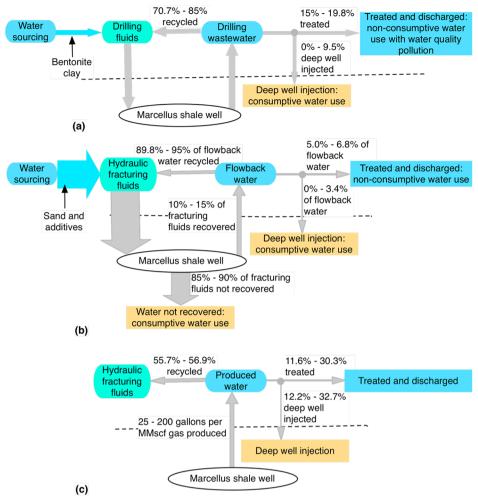


Figure 2. Direct consumptive and nonconsumptive water use over the life cycle of a Marcellus shale gas well. Percentages of direct wastewater management options under the current situation in Pennsylvania are shown for (a) drilling wate, 6,52 (b) hydraulic fracturing water, 2,5,52 and (c) produced water. 52,53

throughout the life span of the well. For the well production phase, gas processing and transmission are included in the model while gas utilization is outside the analysis boundaries. When gas production drops in a well, restimulation through hydraulic fracturing may be used; however, this is not included in the present model as it is likely that only a minority (15%) of the Marcellus shale wells have restimulation potential. Well closure is performed at the end of the well life span, including procedures of well plugging, site restoration, and equipment removal, 32 and these are included in the analysis.

Direct and Indirect Water Use. Direct water use refers to water used at the well site mainly for well drilling and hydraulic fracturing. Indirect supply chain water use during well pad construction is for infrastructure components production and energy consumption. During well drilling and hydraulic fracturing, indirect water is used for producing drilling mud, fracturing proppant, and additives. Water is also indirectly used for production of diesel fuel consumed in drilling and pumping equipment. In addition, generation and trucking of supply water and trucking and management of well wastewater have associated indirect water use. Additionally Gas production, processing, and pipeline transmission consume energy and result in indirect water use. For well closure, water is indirectly used for land reclamation, plugging materials

and energy consumption. Table S1, Supporting Information, summarizes the direct and indirect water use activities.

Consumptive and Nonconsumptive Water Use. Consumptive water use refers to the water evaporated during production, lost underground, or embodied in a product; it results in a net loss of water in the watershed where the water originates and reduces the water availability of that region. Nonconsumptive water use denotes the water that is returned after use to the watershed where it originates; it may generate wastewater and result in degradation of water quality of the water region and/or increased costs to treat wastewater. 46–48

Figure 2 illustrates the direct water life cycle and water consumption for Marcellus shale well development. Direct water life cycle starts from the water withdrawals from different sources: freshwater withdrawn from surface or groundwater sources or purchased from public water suppliers, and wastewater recycled from produced water or other wastewater. ^{6,49,50} Water purchased from public water supply (20% of the freshwater withdrawal in Pennsylvania) has direct and indirect water use impacts since the water has been treated, and the untreated surface water (80% of the freshwater withdrawal in Pennsylvania) only has direct water use impacts. ^{49,51} A minimal percentage of water is withdrawn from groundwater in Pennsylvania, and thus, it is not considered in the study. After water is trucked to the well pad and stored the drilling and

hydraulic fracturing fluids are produced on site with addition of chemical additives and sand. After use, drilling fluids and some of the fracturing fluids return to the surface as drilling wastewater and flowback water. The fracturing water that is not returned is considered to be consumed.² Wastewater disposed of via deep well injection is also considered as consumptive water use.

APPROACH AND DATA SOURCES

Hybrid LCA Model. In this study, a hybrid LCA model was developed, which combined process-based LCA and economic input—output (EIO-LCA). The process-based LCA approach was applied for direct life cycle water use impacts, while the EIO-LCA model was used for indirect supply chain water use impacts. Indirect water withdrawal and consumption was differentiated among U.S. economic sectors. The framework of the hybrid LCA model is shown in Figure S1, Supporting Information.

Scenarios Evaluated. In this study, four scenarios are defined based on different management options of Marcellus shale well flowback and produced water.

- (1) Current conditions in Pennsylvania. Currently, Marcellus shale flowback and produced water can be reused, treated, or disposed of via deep well injection. The percentages of these management options are shown in Figure 2, which were obtained from various studies in 2011–2013.
- (2) Complete discharge. The theoretical case where all Marcellus shale well flowback and produced water are assumed to enter the environment. Direct discharge of oil and gas produced water is prohibited by federal law; ⁵⁶ this case is developed to assess the maximum potential toxicity of Marcellus shale flowback and produced water. It is also used to identify the chemical species in flowback and produced water with the largest environmental toxicity, enabling improved design of wastewater treatment.
- (3) Direct reuse and desalination. All flowback water is recycled with minimum treatment, and all produced water is treated via desalination to preuse level.
- (4) Complete desalination. All flowback and produced water are treated via desalination to preuse level. Extensive treatment is used in this scenario to remove all pollutants of concern in both flowback and produced water (e.g., salts and NORM), and the water quality pollution impacts from Marcellus shale flowback and produced water are minimized.

Direct Water Consumption. The drilling process requires 300–380 m³ of water per well, with a median of 320 m³ per well, either from recycled drilling wastewater or freshwater withdrawal. For hydraulic fracturing, a direct water use inventory was compiled based on well completion reports submitted to the Pennsylvania Department of Environmental Protection (PADEP) in 2010. We fitted a normal distribution to the freshwater withdrawal volumes, which indicates that 3500–26 000 m³, with an average of 15 000 m³ of water, is required to hydraulically fracture a single well in the Marcellus shale formation in Pennsylvania. We consider 88–90% of the hydraulic fracturing makeup water to be freshwater, and the balance is from recycled flowback water and other wastewater. On the basis of the water requirement information and percentages of wastewater management as

shown in Figure 2, we assessed direct water consumption of a Marcellus shale well under current conditions in Pennsylvania.

Indirect Water Consumption. Well operation parameters of a Marcellus shale well were obtained from various data sources (see Tables S2 and S3, Supporting Information) for cost estimation of supply chain production, and calculation details for cost estimation are provided in the Supporting Information. Indirect water use was assessed with the EIO-LCA model based on the cost estimation. S5 Indirect consumptive water use and nonconsumptive water use for different economic sectors were distinguished using their corresponding water consumption coefficients obtained from various studies. 18,60–63

Water Scarcity Impact of Water Consumption. A challenge of using LCA for water use impacts is the local nature of water impacts. Consuming the same amount of water has different effects in watersheds with different water availability. In this study, locational variation of direct water consumption is considered by grouping the water use information into Ohio River Basin (ORB) wells and Susquehanna River Basin (SRB) wells in Pennsylvania based on well geographical information. Findirect supply chain water consumption was also estimated for wells in the two basins, respectively, based on their regionalized water use and well depth information. Figure S2, Supporting Information, shows the regionalization map.

Life cycle water consumption impacts were quantified with the water scarcity index (WSI).⁶⁴ Water consumption impact was calculated in eq 1, where WSI is used as an impact characterization factor for water consumption.

water consumption impact (m³/well)

= WSI of watershed i

 \times water consumption in watershed i (m³/well) (1)

In this study, the Aqueduct physical water risk quantity indicator developed by the Water Resources Institute was used as the characterization factor. This indicator ranges from 0 to 5, with a higher score indicating more severe water scarcity problem. The WSI is 2.76 for the SRB and 1.60 for the ORB, indicating that neither is a severely water-stressed area. Although the water source for drilling and hydraulic fracturing is not always known for a given well, the assumption was made that water is sourced from within the same hydrologic basin as the well location. Since geographical information was not available for supply chain production, indirect water consumption impact was quantified with the U.S. national WSI of 2.33. 65,66

Direct Wastewater Generation from Marcellus Shale Well Site. During the drilling process, drilling fluids bring rock cuttings from the well bore to the surface. Solids and liquids are then separated as drilling cuttings and drilling wastewater. All drilling cuttings are assumed to be disposed of in landfills.⁶⁷ Few existing studies are available for toxic pollutant concentrations in drilling wastewater; thus, for the present analysis it is assumed that chemicals in drilling wastewater have minimal direct water quality pollution impacts. For flowback and produced water, Hayes (2009) reported on water quality at 19 wells sampled from day 1 to day 90 after hydraulic fracturing occurred. 10 These data were evaluated and used in the current analysis as representative of Marcellus shale produced water (see Table S5, Supporting Information, for details on data cleaning and analysis for data sets from ref 10 as well as summary statistical results). Concentrations of water quality

parameters including TDS are summarized in Appendix A of the Supporting Information. These results are consistent with existing water quality studies on Marcellus shale wastewater. As mentioned in the Introduction, other waste fluids from the well site only represent a minimal percentage and thus were neglected in the study.

Impact Assessment of Water Quality Pollution with TRACI. The tool for reduction and assessment of chemical and other environmental impacts (TRACI) was used to quantify the environmental toxicity of chemicals in flowback and produced water under scenario 2 (complete discharge) as well as pollutant loadings from indirect supply chain water use activities under all four scenarios. Specific impact categories in TRACI relevant to water quality pollution are eutrophication potential (in kg of N equivalent), freshwater ecotoxicity potential (in kg of 2,4D equivalent), carcinogenic potential (in kg of benzene equivalent), and noncarcinogenic potential (in kg of toluene equivalent). 69,70 TRACI impact assessment requires a mass-based water pollutant inventory. To obtain these values, the volumes of flowback and produced water were matched to contaminant concentrations from Hayes. 10 Pretreatment pollutant loadings of flowback water within 14 days and produced water after 14 days throughout the well life span were calculated in Appendix B of the Supporting Information. Potential toxicity characterization factors in TRACI were mapped to the chemical species in Marcellus shale wastewater (see Appendix C of the Supporting Information for details). The potential environmental toxicity of indirect supply chain water use activities was assessed using the EIO-LCA model and TRACI characterization factors. 55,70 The TRACI impact assessment method was consistently applied for direct and indirect water quality pollution impacts for freshwater ecotoxicity and eutrophication potential.

Impact Assessment of Water Quality Pollution with Wastewater Treatment Cost. TRACI analysis accounts for the potential toxicity of the wastewater, but it is not an adequate representation of all possible impacts. Few characterization factors are available in TRACI for salts like chloride and bromide and for radioactivity. However, studies have shown that high-salinity waters may result in ecotoxicity effects (e.g., refs 17, 72, and 73). Also, carcinogenic disinfection byproducts in drinking water systems may be caused by elevated bromide level in source water. 17,74,75 Only a limited number of studies have investigated the potential ecotoxicity of NORM, and these studies indicate that the environmental toxicity of NORM from gas-produced water might be negligible. To account for these impacts we use wastewater treatment cost as an additional characterization factor for Marcellus wastewater pollution impacts. Wastewater treatment processes such as desalination include removal of salinity and NORM. This proposed impact assessment method provides a relative impact indicator of Marcellus shale well wastewater pollution, rather than predicting absolute cost of wastewater management. The logistic cost for transportation of wastewater is not included in the cost estimate; rather, we focus on the treatment costs as these demonstrate the differences associated with different treatment options.

Wastewater treatment costs were assessed for all four defined scenarios. Different treatment options are available for Marcellus shale well flowback and produced water, and treatment cost varies with different goals for end point of water quality. The cost of reuse of produced water is reported to range from 36 to 63 cents/m³ of produced water in 2012,⁷⁷

which includes some primary treatment such as settling or filtration to remove suspended solids. Deep well injection cost varies from 0.59 to 13 dollars/m³ of produced water in 2012. As Comprehensive treatment of produced water for subsequent surface water discharge requires desalination to meet requirements for discharge (TDS of 500 mg/L in Pennsylvania As). Thermal desalination (typically required for very high TDS waters from shale development) is reported to cost 53–71 dollars/m³ of produced water in 2012, including treatment and residual disposal.

Uncertainty and Sensitivity Analysis. Information on direct fracturing water use, well depth, and pretreatment pollutant loadings in flowback and produced water was obtained for individual Marcellus shale wells from actual well operations⁵⁹ and experimental data.¹⁰ Probability distributions were fitted to the data to account for data variability (Table S3, Supporting Information). Mean and range values of other model parameters were acquired from different literature, based on which uniform, triangular, or discrete distributions were defined (Table S3, Supporting Information). To account for model uncertainty, the Monte Carlo method was used by running the model 10 000 times with the model parameter values sampled randomly from their probability distributions. Further, a sensitivity analysis was performed on the life cycle water consumption per well and per MJ of gas by changing the model parameters by $\pm 10\%$ from their base case values under current conditions in Pennsylvania, and the top 10 influential model parameters were identified.

RESULTS

Local Water Consumption Impact under Current Conditions in Pennsylvania. Estimated from the raw data, ⁵⁹ a well in SRB has directly consumed 5100–22 000 m³ (13 000 m³ on average) of water while a well in ORB has directly resulted in 610–22 000 m³ (11 000 m³ on average) water consumption. Water scarcity impact results indicate that direct water consumption of a well in SRB (14 000–60 000 equivalent m³) has a higher water stress impact than a well in ORB (980–36 000 equivalent m³). Indirect water consumption was estimated to be 4700–12 000 m³ (averagely 8000 m³) per well for SRB and 3500–12 000 m³ (averagely 7700 m³) per well for ORB. Water scarcity impact of indirect water consumption for a well in SRB (11 000–28 000 equivalent m³) is close to a well in ORB (8200–29 000 equivalent m³).

Direct and Indirect Life Cycle Water Consumption under Current Conditions in Pennsylvania. Direct water consumption for drilling and fracturing for an average Pennsylvania Marcellus shale well was estimated to be 12 000 m³ (2600 to 21 000 m³). Total indirect water consumption was estimated to be 7900 m³ (4100–12 000 m³) per well with disaggregation among different U.S. sectors. The top five indirect water consumption sectors are listed in descending order: grain farming, sand mining, power generation and supply, nonresidential structures, and all other crop farming (Figure S4, Supporting Information). Grain farming is likely related to organic chemical production for fracturing additives. So Sand mining might be for proppant production. A3,79 In our study, an average national electricity grid is assumed for power generation throughout the supply chain, while water use for power generation may vary significantly from one region to another.

Direct and indirect water consumption across the life cycle stages of a Marcellus shale well is shown in Figure 3. Well

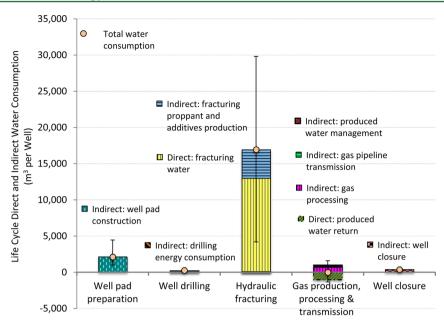


Figure 3. Estimated life cycle direct and indirect water consumption for a Marcellus shale gas well. Error bars represent the limit of the 90% confidence intervals of water consumption from each life cycle stage, which accumulate the uncertainties of all model parameters. Numeric data are provided in Table SD2 of Appendix D, Supporting Information.

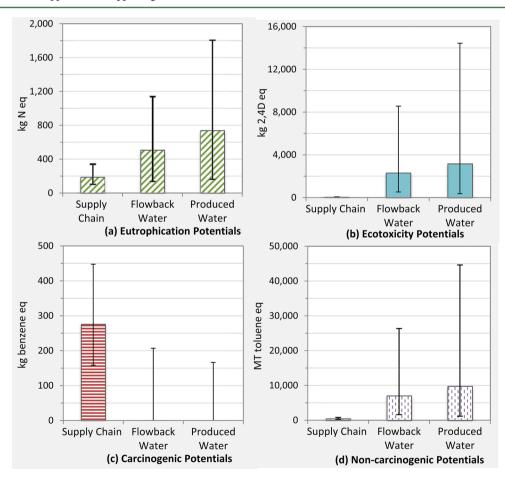


Figure 4. Potential environmental toxicity of supply chain production, flowback, and produced water of a Marcellus shale gas well under complete discharge scenario. Median values are shown with error bars representing the minimum and maximum estimates based on water quality experimental results of wastewater samples from 19 individual Marcellus shale wells over 90-day period post hydraulic fracturing.

hydraulic fracturing is the largest water consumption stage, representing 86% of the total freshwater consumption across

the life cycle of Marcellus shale well excluding gas utilization. Seventy-six percent of the water consumption during the hydraulic fracturing phase is direct water consumption for fracturing fluids, while the balance (24%) is indirect water consumption primarily for sand and additives production. Direct water consumption for drilling is very small since drilling requires much less water than fracturing, and most of the drilling water is recycled within the production system. Well pad preparation is the second largest water consumption life stage, which results in 11% of the total water consumption, almost entirely indirect consumption for construction. Production, processing, and transmission of shale gas have nearly zero net water consumption because the produced water generated over the life of the well offset the indirect water use for supply chain production after treatment and discharge. Fuel consumed for drilling and fracturing operations contributes a relatively small proportion of the life cycle water consumption per well. Water/wastewater transport, public water supply, and wastewater management have very small associated water consumption. If refracturing is considered 3 times per well over a 30-year life span as in Clark et al., 16 life cycle water consumption would be increased from 20 000 to 54 000 m³ per well; however, as noted above, the potential for refracturing in Marcellus wells may not be expected to be very high.³¹

TRACI Toxicity Analysis of Water Quality Pollution under Complete Discharge Scenario. Life cycle TRACI analysis results for the complete discharge scenario are shown in Figure 4. For comparison purposes, potential toxicity of supply chain production, flowback, and produced water are shown separately for each impact category. Despite the large uncertainties, the results indicate that the potential toxicity of the direct wastewater generated during Marcellus shale well development is more of a concern than the water quality pollution impacts across the supply chain.

The eutrophication potential of Marcellus shale well flowback and produced water (assuming no treatment) resulted from the high chemical oxygen demand (COD) of the wastewater. A single component, barium, accounts for over 90% of the ecotoxicity potential from the flowback and produced water. Other major chemicals with freshwater ecotoxicity impacts are identified as zinc, methanol, pyridine, lead, toluene, and acetone in descending order. As noted previously, the salinity of flowback and produced water would likely contribute to additional ecotoxicity potential but is not included in TRACI. In terms of carcinogenic potential, pyridine, lead, benzene, toluene, bis(2-ethylhexy)phthalate, and 1,2,4-trimethylbenzene in Marcellus shale flowback and produced water are identified as major contributors, but the overall mass of these constituents in flowback and produced water is very low. 10,111 Although Figure 4c shows that Marcellus shale well flowback and produced water have low potential carcinogenic impacts, NORM and salts (chloride/bromide) might have some potential toxicity that are not assessed in the TRACI analysis. Noncarcinogenic potentials are mainly caused by barium, zinc, pyridine, methanol, lead, acetone, bis(2ethylhexy)phthalate, toluene, and benzene; barium dominates the noncarcinogenic effects.

Wastewater Treatment Cost of Marcellus Shale Well Wastewater under the Four Scenarios. Table 1 summarizes the treatment cost of Marcellus shale well wastewater over the well life span under the four scenarios defined in the method section. Under scenario 2 (complete discharge), no treatment is performed for Marcellus shale well flowback and produced water, and thus, only the treatment cost of drilling wastewater was accounted for . However, the direct potential

Table 1. Water Quality Pollution Impact Assessment Using Wastewater Treatment Cost under the Four Case Scenarios^a

	mean		90% CI-L		90% CI–U	
wastewater treatment cost	\$/well	\$/TJ gas	\$/well	\$/TJ gas	\$/well	\$/TJ gas
scenario 1 (current conditions in Pennsylvania)	24 000	8.9	9800	3.4	49 000	17
scenario 2 (complete discharge)	2800	1.3	1500	0.3	4200	3.4
scenario 3 (direct reuse and desalination)	65 000	20	13 000	6.7	160 000	34
scenario 4 (complete desalination)	150 000	60	59 000	19	270 000	130

"Note: 90% CI-L and 90% CI-U are the lower and upper bound of the 90% confidence interval of the wastewater treatment cost estimates.

water quality pollution impacts are large as assessed in the previous section. When more treatment is used from scenario 2 to other scenarios, the cost is increased and the potential environmental toxicity of indirect water use is slightly increased due to more intensive treatment processes (Figure S6, Supporting Information), while direct wastewater pollution impacts are reduced. Although both scenario 3 (direct reuse and desalination) and scenario 4 (complete desalination) have minimal direct wastewater pollution impacts, the former is preferable to the latter since less wastewater treatment cost is required.

The wastewater cost per trillion joule (TJ) of gas produced was also calculated in Table 1 as an indicator relating the performance of current Marcellus shale well wastewater treatment technologies with production of natural gas. When the gas production rate is low and/or the produced water generation rate is high, the cost impact indicator is high. When the gas production rate is high and/or the produced water generation rate is low, the cost impact indicator is low.

Incorporating Uncertainty in Gas Production. High uncertainty exists in the ultimate gas reserve per well¹ and would affect the life cycle water consumption and TRACI impacts per MJ of gas. Direct and indirect life cycle water consumption was estimated to be 0.0017–0.026 L/MJ of gas with an average of 0.0094 L/MJ of gas. Water consumption for each well life stage and the water quality pollution impacts per MJ of gas are summarized in Tables S9 and S10, Supporting Information.

DISCUSSION

A life cycle perspective is important to assess the water impacts of a Marcellus shale gas well. The uncertainties in the estimation results are mainly introduced by the variability of water use by different well operators and the variability of water quality parameters of Marcellus shale flowback and produced water. The results of the sensitivity analysis, shown in Figures S7 and S8, Supporting Information, indicate that water use for hydraulic fracturing, ultimate gas reserve per well, water consumption for proppant, and additives production are the most influential factors on the life cycle water consumption per well or per MJ of gas produced. Other factors have a relatively small impact on these results with the same percentage of change.

Gas utilization for power generation, although out of our study scope, may require substantial amounts of water for

cooling the stream engines (e.g., ²⁴). The end use phase, if included, would dominate the life cycle water consumption for Marcellus shale gas and represent a large fraction of water consumption. Water consumption for gas utilization has been studied in a variety of literature reports (e.g., refs 22 and 24) and could be added to the estimation result of this study to obtain the whole life cycle water consumption for Marcellus shale gas. End use could also result in chemical water vapor generated from gas combustion; however, this water vapor is not available immediately to downstream users in the well development region where water is withdrawn. Water quality pollution impacts from the end use of shale gas are minimal since gas utilization typically generates little wastewater.

The actual direct water quality pollution impacts are likely between the complete discharge scenario, which is not permitted by law, and the complete desalination scenario, which is very costly, because some produced water has historically been partially treated and released to surface waters in Pennsylvania.⁵³ In our study, TRACI toxicity analysis on direct water quality pollution impacts was only conducted for the complete discharge scenario, but it could also be performed for the current conditions scenario if data on post-treatment water quality of Marcellus shale well wastewater were available. Although currently TRACI toxicity analysis has not captured impacts of salts and NORM, we developed the life cycle inventory of pollutant concentrations and loadings from Marcellus flowback water and produced water (as in Appendix A and Appendix B of the Supporting Information). Future studies can make use of this inventory to quantify the toxicity of salts and NORM once their impact characterization factors are developed in TRACI or other life cycle impact assessment methods.

The method of using wastewater treatment cost as an additional impact indicator for water quality pollution is efficient for assessing direct wastewater pollution impacts from Marcellus shale gas well. Future studies could be performed to assess treatment cost for wastewater generated from indirect supply chain production. For example, wastewater cost could be obtained for different U.S. sectors on the basis of per volume of wastewater generated. With the EIO-LCA model and water consumption coefficients, water withdrawal and water consumption could be estimated. The difference between these two estimates could be considered as the volume of the wastewater generated from various U.S. sectors. Combining the wastewater costs for different U.S. sectors and wastewater generated from these sectors, the treatment cost of wastewater generated from supply chain production could be estimated.

ASSOCIATED CONTENT

S Supporting Information

Additional tables, figures, and detailed documentation of calculation, data cleaning, and processing regarding Marcellus shale well produced water quality and the process of mapping TRACI characterization factors with chemical substances in Marcellus shale well flowback and produced water. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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