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Formation of disinfection by-products under influence of shale gas produced water

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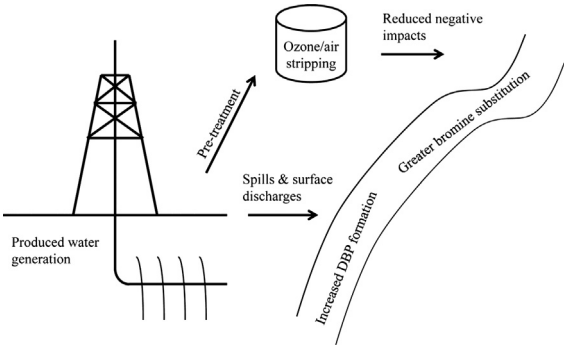
HIGHLIGHTS

- Formation and speciation of DBPs under influence of produced water were quantified.
- Measurable alterations to DBP formation were identified at a blend ratio of 0.005%.
- A shift to a more bromine substitution direction was found at increased blend ratio.
- Ozone/air stripping of produced water reduced the formation of brominated DBPs.
- DBP formation was affected by background NOM in produced water – impacted waters.

GRAPHICAL ABSTRACT



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ABSTRACT

Accidental spills and surface discharges of shale gas produced water could contaminate water resources and generate health concerns. The study explored the formation and speciation of disinfection by-products (DBPs) during chlorination of natural waters under the influence of shale gas produced water. Results showed the presence of produced water as low as 0.005% changed the DBP profile measurably. A shift to a more bromine substitution direction for the formation of trihalomethanes, dihaloacetic acids, trihaloacetic acids, and dihaloacetonitriles was illustrated by exploring the individual DBP species levels, bromine substitution factors, and DBP species fractions, and the effect was attributable to the introduction of bromide from produced water. The ratio of dichloroacetic and trichloroacetic acids also increased, which was likely affected by different bromination degrees at elevated bromide concentrations. Increasing blend ratios of produced water enhanced the formation of DBPs, especially the brominated species, while such negative effects could be alleviated by pre-treating the produced water with ozone/air stripping to remove bromide. The study advances understandings about the impacts of produced water spills or surface discharges regarding potential violation of Stage 2 DBP rules at drinking water treatment facilities.

1. Introduction

Shale gas, as an unconventional resource, becomes an increasing share of the energy portfolio in the United States and many other countries nowadays. Along with the benefits of increased domestic oil and gas production, the shale gas boom also leads to substantial

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environmental concerns (Vidic et al., 2013). The increased activities in exploration, drilling, and shale gas production have generated large volumes of produced water that need to be properly handled, overwhelming the capacity of current wastewater disposal infrastructures (Lutz et al., 2013). For areas where disposal of shale gas produced water is not permitted locally, transportation of the wastewater to longer distances become the only option, imposing a risk of spills from vessel and pipeline leaks and truck overflows (Shrestha et al., 2017). Lauer et al. (2016) reported nearly 3900 spills during transportation of produced water to underground injection wells since 2007, and the pipeline leaks contributed to the highest number and largest volume of those spills. An increasing trend of such spills during the transportation can be expected with the growth of industry and co-evolving of regulations.

Water quality concerns rise from contamination of water sources by those spills and surface discharge of inadequately treated produced water. The elevated level of organic compounds (from chemicals injection during drilling or fracturing) and elevated salinity due to extremely high concentrations of total dissolved solids (TDS) in produced water (e.g. up to 400,000 mg/L TDS in Williston Basin, North Dakota (Harkness et al., 2015)) are typical concerns in negatively impacted water sources. The overall increase of salinity in some watersheds has been associated with a relatively high frequency of spills according to Harkness et al. (2015). Although dilution with freshwater reduces instream concentrations of the TDS, a study still reported 2–10 fold higher chloride concentrations and 40 fold higher bromide concentrations compared to the background level at a distance of 1.7 km downstream from the discharge site (Warner et al., 2013). In addition, sediment contamination far downstream was also detected and it persisted for long periods of time (Burgos et al., 2017). Since a relatively small volume of spill or discharge of produced water has measurable impacts on water quality, further investigation is needed to discern those impacts.

Recent studies explored the environmental implications of disinfection by-product (DBP) formation in produced water – impacted water sources (States et al., 2013; Parker et al., 2014; Hladik et al., 2014). Those studies are important for water industry, because the polluted waters will eventually go through water treatment processes at publicly owned treatment works (POTWs), which involve a disinfection step before consumers. Since the formation of DBPs depends on a variety of factors such as organic and inorganic precursors, disinfectant level, and other operational factors, the mixtures and types of DBPs formed from these water sources can be quite different from those found in a non-polluted drinking water source due to the unique signatures of chemical composition in produced water. For instance, organic DBP precursors originating from produced water could be traced back to the chemicals used in hydraulic fracturing, which are characterized as saturated aliphatic compounds and a small fraction of aromatic, resin, and asphaltine compounds (Shrestha et al., 2017). Inorganic precursors originating from produced water include bromide (McTigue et al., 2014) that leads to the formation of more toxic brominated DBPs (Cowman and Singer, 1996) and various ions (e.g. ferric, calcium) that affect the DBP formation mechanisms (Liu et al., 2011; Zhao et al., 2016; Szczuka et al., 2017). The increase of these constituents of concern in produced water – impacted water sources imposes a greater challenge for water utilities, because it could affect the ability of POTWs drawing water from these sources to comply with the Stage 2 DBP rules. In the meanwhile, development of methods for reducing the impacts of bromide on DBP formation is under way. Notable efforts include investigations on combined electrolysis and volatilization for bromide removal and DBP control from drinking water by Kimbrough and Suffet (2002, 2006, Kimbrough et al., 2012), although its applicability in produced water is largely unknown. Sun et al. (2013) worked on produced water research with a purpose of selective oxidation of bromide to bromine. It appears the direction towards conversion of bromide to bromine followed by bromine removal from produced water is promising for DBP control. On the other hand, as the DBP formation upon chlorination of the produced water – impacted water sources might be under the influence of other substances in produced water, the scenario could be more complicated.

To protect consumers from negative health impacts, formation of DBPs under the influence of produced water should be adequately studied. For instance, conventional produced water treatment is neither designed nor successful in removing halides by process series of chemical precipitation, flocculation, and solids separation (Harkness et al., 2015); consequently, there could be significant impacts on DBP formation as a result of increased bromide level, because the dosing of chlorine at POTWs will oxidize bromide into hypobromous acid, which is up to twenty times more reactive than hypochlorous acid in the formation of regulated DBPs (Landis et al., 2016). Identification and quantification of DBPs under various chlorination scenarios in presence of produced water are needed. Yet, studies about examining DBP formation and speciation in such scenarios are not sufficient, and the roles of produced water constituents in DBP formation are also not very clear. In this study, we filled the research gap by exploring the effects of produced water on the formation and speciation of DBPs under various produced water – impacted scenarios. For POTWs drawing water from produced water – impacted water sources with an increasing risk of violating the Stage 2 DBP rules due to the complex chemical constituents of produced water, the study would be of great importance. In addition to varying the blend ratios to mimic the produced water impact at various degrees, the distribution of DBP species and bromine substitution factors (BSFs) of different classes of DBPs were also analyzed. Moreover, a pre-treatment approach with ozone/air stripping, which was aligned with the direction of converting bromide to bromine, was used to remove bromide from the produced water, and such strategy was also evaluated to minimize the impacts of produced water on DBP formation. While the development of unconventional gas resource is facilitated by technology innovation, the study advances understandings about the impacts of produced water spills or discharges regarding potential violation of DBP rules during treatment of the produced water – impacted water sources.

2. Materials and methods

2.1. Chemicals

Trihalomethane (THM) Calibration Mix containing trichloromethane (TCM), bromodichloromethane (BDCM), chlorodibromomethane (CDBM) and tribromomethane (TBM) (100 μg/mL each component in methanol), EPA 552.2 Haloacetic Acids (HAAs) Mix containing monochloroacetic acid (MCAA), monobromoacetic acid (MBAA), dichloroacetic acid (DCAA), trichloroacetic acid (TCAA), bromochloroacetic acid (BCAA), dibromoacetic acid (DBAA), bromodichloroacetic acid (BDCAA), chlorodibromoacetic acid (CDBAA), and tribromoacetic acid (TBAA) (2000 μg/mL each component in methyl tert-butyl ether (MTBE)), EPA 551B Halogenated Volatiles Mix containing dichloroacetonitrile (DCAN), trichloroacetonitrile (TCAN), bromochloroacetonitrile (BCAN), dibromoacetonitrile (DBAN), 1,1-dichloro-2-propanone (1,1-DCP), 1,1,1-trichloropropanone (1,1,1-TCP), and trichloronitromethane (TCNM) (2000 μg/mL each component in acetone), and chloral hydrate (CH, 1000 μg/mL in acetone) were obtained from Supelco (Bellefonte, Pennsylvania, USA). All other chemicals were of ACS reagent grade purity unless noted otherwise.

2.2. Produced water and its mixing with natural waters

Produced water was synthesized in laboratory based on representative shale gas produced water characteristics summarized by Warner et al. (2013). Chemicals used for the synthesis included sodium chloride (1220 mM), sodium bromide (9.3 mM), sodium sulfate (0.22 mM), calcium chloride (241 mM), magnesium chloride hexahydrate (44.0 mM), barium chloride (12.4 mM), and strontium chloride hexahydrate