Identifying persistent, mobile and toxic (PMT) organic compounds detected in shale gas wastewater

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HIGHLIGHTS

- 162 organic compounds detected in FPW were included in our PMT screening list
- 22 FPW substances are "PMT/vPvM" or very likely meet the criteria
- PMT/vPvM in FPW should be prioritized to protect regional water resources

GRAPHICAL ABSTRACT
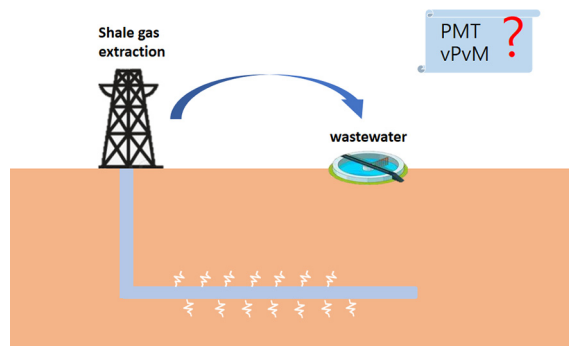
ARTICLE INFO

ABSTRACT

Shale gas exploitation is a water-intensive process, generating flowback and produced water (FPW) with complex chemical compositions. Reuse, disposal and treatment of FPW are of increasing concern, because of the potential risk of FPW contamination to the surrounding aquatic environment and drinking water sources when emitted. Among numerous organic substances present in FPW, of particular concern are those that are persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM). PMT and vPvM substances have the greatest potential to spread in groundwater and are the hardest to remediate. This study presents the outcome of a literature review to identify organic compounds that were previously detected in FPW. The 162 target compounds identified from this review were assessed to see if they can be considered PMT/vPvM substances based on their substance properties. Our results indicated that most FPW substances are "not PMT", accounting for 108 (66.7 %) compounds. In total 22 FPW substances can be considered PMT/vPvM or very likely to meet this criteria if more data were available. Examples of PMT substances in FPW include anthracene, 1,4-dioxane and 1,4-dichlorobenzene. PMT/vPvM compounds identified in FPW should be prioritized for risk management measures and monitoring in order to protect regional water resources.

1. Introduction

Natural gas extraction is considered a transitional energy source from coal and petroleum towards decarbonization, until environmentally sustainable, renewable energy sources are more widely available (Pacala and Socolow, 2004; Vidic et al., 2013; Zhong et al., 2021). To this end, advances

in hydraulic fracturing and horizontal drilling techniques have rapidly accelerated gas and oil extraction from shales. Production of shale gas continues to surge in many countries. For instance, shale gas production increased by eightfold in the U.S. from 2007 to 2016 (Kondash et al., 2018). China owns one of the most abundant shale gas resources in the world (Ni et al., 2018; Yu et al., 2016; Zhong et al., 2021), causing shale gas exploitation to boom in China in the last decade (Zou et al., 2021). However, the potential impacts on local environment quality caused by shale gas production has been drawing increasing concern by the public and researchers (Adgate et al., 2014).

In order to better ascertain key environmental impacts from shale gas extraction that researchers have focused on, a literature search was conducted by searching the Web of Science Core Collection database using the following keywords: "(shale gas OR hydraulic fracturing) AND (environment OR environmental) AND (chemical OR chemicals)", which resulted in 1632 studies (https://www.webofscience.com, accessed on May 11th 2022). As a next step, the co-occurrence of terms in titles and abstracts were analyzed using VOSviewer (http://vosviewer.com). Fig. 1 presents four clusters of research focus. The red cluster consists of the terms "hydraulic fracturing", "chemicals", "wastewater", "disposal", "contamination" and "treatment", indicating that environmental impacts from water contamination was the most common research topic among the hydraulic fracturing literature. Other clusters that were less commonly linked with hydraulic fracturing include hydrogeology (yellow), petroleum geology (green) and technological challenges (blue). This research focus on water contamination is not surprising, considering that shale gas extraction is a water and chemical intensive process, requiring massive freshwater consumption and a complex array of chemicals (Jin et al., 2022). In the context of climate change and drought, it is a concern that water consumption from hydraulic fracturing could intensify water stress, both in terms of quantity and quality (Yu et al., 2016). The complex chemical composition of generated wastewater, disposal, treatment and reuse of the wastewater collectively pose unknown risks to the surrounding water environment (Elsner and Hoelzer, 2016; Liu et al., 2020).

Protecting water resources from the contamination of persistent, mobile and toxic (PMT) substances, as well as very persistent and very mobile (vPvM) substances, is of primary importance for protecting regional water resources. PMT/vPvM substances have long environmental half-life values, an intrinsic propensity to reach drinking water extraction points, and are commonly difficult to remove during water treatments (Hale et al., 2020a; Hale et al., 2020b; Jin et al., 2020). Numerous PMT substances have already been identified in different water bodies (Huang et al., 2021; Schulze et al., 2019a; Zahn et al., 2019). Detection of PMT/vPvM substances is often a challenging task owing to many of them being very highly polar or ionic (Reemtsma et al., 2016; Schulze et al., 2019a; Zahn et al., 2019), for which advanced analytical tools are required for both target and non-target analysis. A focus of this study is to identify the PMT/vPvM substances present in the flowback and produced water (FPW) from hydraulic fracturing.

FPW refers to the wastewater generated and returned to surface during shale gas production (Chen and Carter, 2017; Rosenblum et al., 2017). FPW contains various organic and inorganic compounds, including chemical additives for hydraulic fracturing, geogenic organic compounds and transformation products (Hoelzer et al., 2016; Rosenblum et al., 2017). An increasing number of studies have attempted to characterize chemical compositions in the FPW, and several toxic organic compounds such as 1,4-dioxane, anthracene, nitroaniline, and benzo(*a*)pyrene were identified (Danforth et al., 2020). However, the variety of organic compounds that can be considered PMT/vPvM has not yet been assessed, but these should be prioritized due to their hazardous properties for human health and the environment. To fill this gap, the main goal of this study is to identify and classify PMT/vPvM substances among the detected organic compounds in FPW. The purpose of this list would be to provide useful information to support risk-based management of chemicals and pollutants associated with shale gas extractions.

2. Methods

2.1. Compounds screening list

A literature review was conducted by searching the research papers associated with FPW during hydraulic fracturing from the ISI Web of Science (see Table S1). Organic compounds detected and identified in FPW, including hydraulic fracturing chemicals, geogenic compounds and transformation products, were extracted from this literature. In total 162 organic pollutants were included (see Table S2).

2.2. PMT assessment criteria

The criteria and procedures for the persistency, mobility and toxicity assessments are based on the approach developed in the previous studies (Arp and Hale, 2019; Arp and Hale, 2022). Briefly, for the assessment of persistent (P) and very persistent (vP), half-life times of 40 days and 60 days in fresh water are used as the cut-off values, respectively. When half-life data in fresh water data are not available, half-lives in soil and sediment at 120 and 180 days can be used instead (Arp and Hale, 2019). Experimental half-life data are obtained from PubChem Database (NIH, 2020) following the individual query by assessing half-life values for substance biodegradation. However, experimental data are often rare, and thereby results from standardized tests such as inherent biodegradation tests and readily biodegradation tests are adopted to draw not persistent (not P) conclusions. As for compounds missing the above mentioned information, the predicted results using the P Predictor in QSAR Toolbox (OECD, 2020) or EPI Suite (US EPA, 2015) models BIOWIN1–6 and were utilized for P estimations on a weight-of-evidence basis. To express uncertainty or ambiguity in P/vP related to low quality or screening data, additional categories, "potential P/vP" and "Potential P/vP + +", were introduced to consider different weight-of-evidence for P conclusions. Compounds labeled as "Potential P/vP + +" have more weight-of-evidence to be P or vP than the "Potential P/vP" ones, such as structural similarity (i.e. read-across) to P/vP substances (Table S2).

The mobility assessment is based on experimentally determined log organic carbon - water partition coefficients (log K_{oc}). Compounds with log K_{oc} values below 4.0 or 3.0 at pH 4–9 are assigned as "Mobile (M)" and "very Mobile (vM)", respectively (Neumann and Schliebner, 2019). Otherwise, "not M" conclusions are drawn instead. When experimental log K_{oc} values are unavailable, screening information, including the log octanol-water partition coefficient (log K_{ow}) for neutral compounds or the pH-dependent octanol-water distribution coefficient (log D_{ow}) for ionizable compounds, are used as a weight-of-evidence assessment for M-conclusions. Specifically, a cut-off value of 4.5 for log D_{ow} (between pH 4–9) is used as an indicator of mobility (M). Experimental data of log K_{oc} or log K_{ow} values were obtained from the PubChem database, while D_{ow} values at different pH values were acquired by using ChemAxon software. In order to address borderline M cases based on log K_{ow} or log D_{ow}, a category "potential M/vM" was introduced when a substances log K_{ow} or log D_{ow} are determined between certain ranges (i.e. below 4.5 and 3.5, respectively), depending on the type of substance and availability of experimental log K_{ow} or log D_{ow} data for certain substances (Arp and Hale, 2019; Arp and Hale, 2022).

The Toxicity (T) assessment is based on criteria used for the PBT assessment within the European REACH Regulation (Annex VIII) with additional considerations specific for drinking water, including carcinogenic category 2, cell mutagenic category 2, and endocrine disrupting properties (Neumann and Schliebner, 2019). Hazard data categories were obtained from the public C&L registry in ECHA website (ECHA, 2020). No observed effect concentrations (NOEC) were acquired from the EnviroTox database (HESI, 2020). If none of the T criteria were met, QSAR Toolbox was used to conduct a Cramer Class assessment (Arp and Hale, 2019), where substances falling into Cramer Class III were considered "Potential T". In case a Cramer Class III was not met, a "not T" conclusion was drawn for the substance.

To make a final PMT/vPvM conclusion (see Fig. 2), a PMT substance had to meet the P (or vP), M (or vM) and T criteria, and a vPvM substance
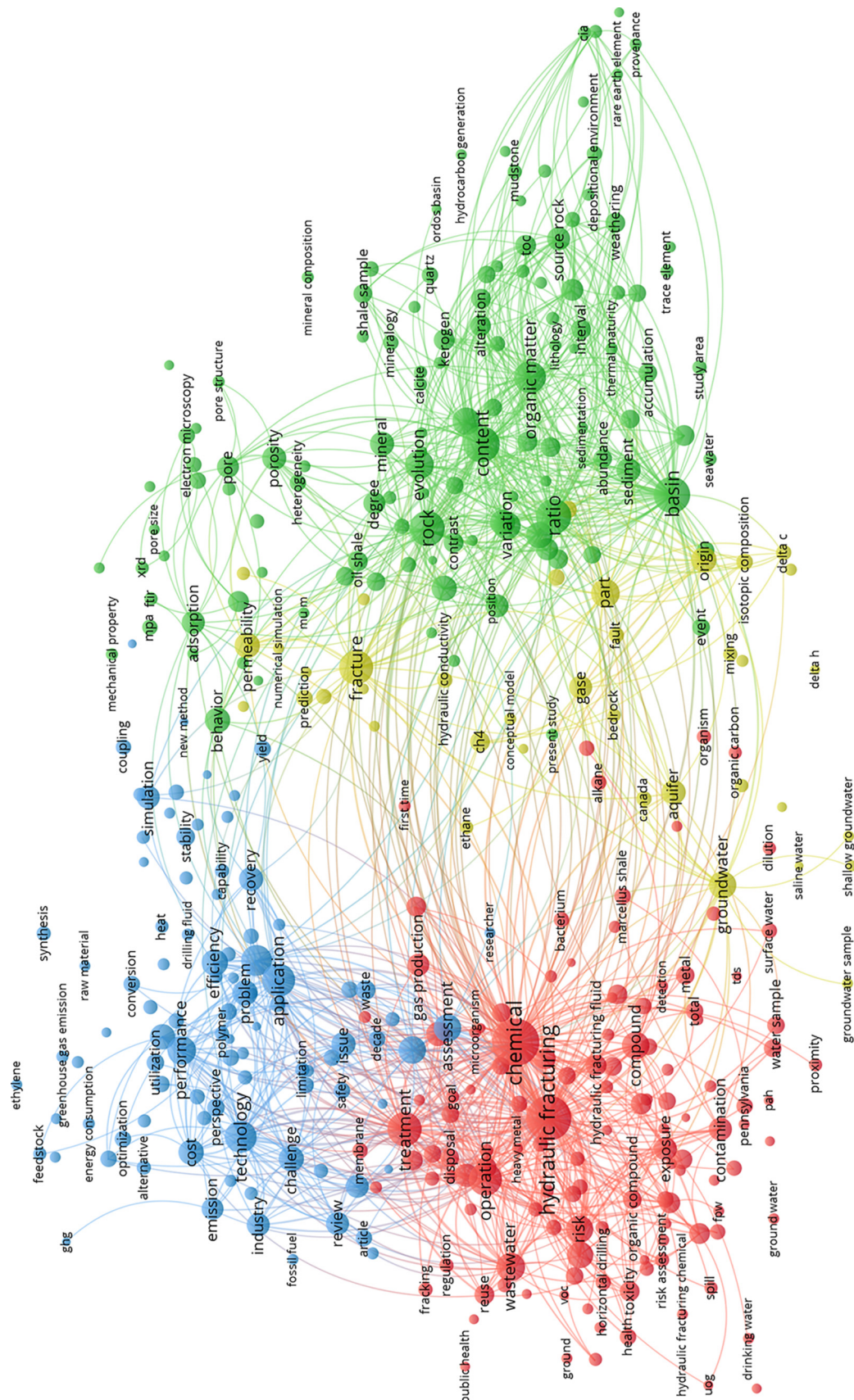
Fig. 1. The network of term co-occurrence in titles and abstracts of the identified research papers on hydraulic fracturing. Different colors represent clusters were the most links occur. The size of the node represents the number of occurrences of the terms. The lines between the nodes indicate the relationship between two terms.
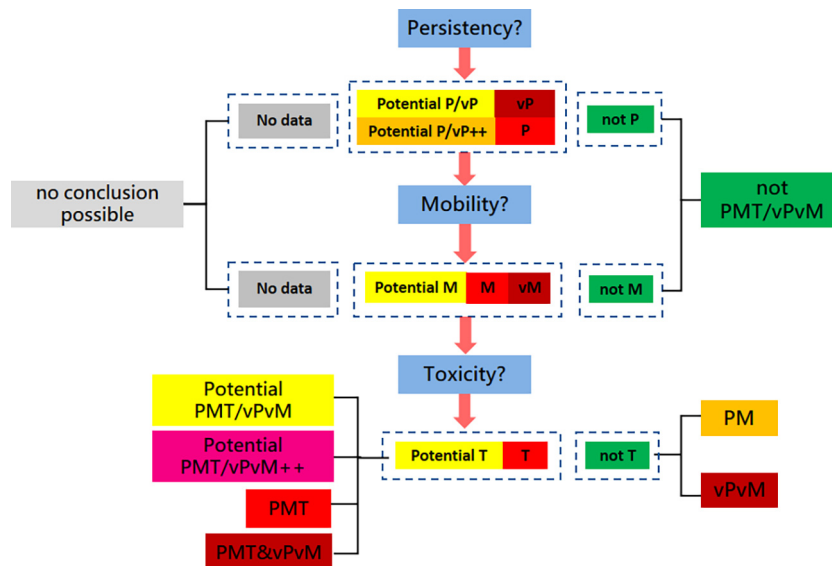
Fig. 2. The standard procedures for PMT screening.

had to meet both vP and vM criteria. Additionally, a weight of evidence "potential PMT/vPvM + +" conclusion is drawn when a compound fall into "Potential P/vP + +" category along with either vM or both M and T (Huang et al., 2021).

3. Results and discussion

3.1. Chemical classification in different scenarios

162 organic compounds were identified in FPW, the majority of them did not fulfil the PMT criteria. In total 108 (66.7 %) substances were considered not PMT (see Fig. 3a, Table S2). The fraction of "Potential PMT/vPvM" substances account for 18.5 % of the 162 substances (see Fig. 3a). Moreover, 15 "potential PMT/vPvM + +" substances were identified, along with two PM substances, four PMT substances, one vPvM substance and two PMT&vPvM substances.

The identified high priority PMT/vPvM substances are presented with their molecular structures in Fig. 4. Chlorinated compounds are common among these, including 1,2-dichloroethane, 1,4-dichlorobenzene, tetrachloroethylene and others. Moreover, small, polycyclic aromatic hydrocarbons (PAHs) and substituted aromatic substances including anthracene, 4-nitroaniline, and 1,2,3,4-tetrahydronaphthalene are also prioritized as PMT or vPvM compounds. Most of the identified PMT/vPvM substances

are suspected hydraulic fracturing additives or their transformation products. However, one of them, anthracene, has also a geogenic origin (Hoelzer et al., 2016). Because the substances meet the PMT/vPvM criteria, special attention should be paid to these substances in order to prevent water contaminations in shale gas field by chemicals, such as by including them in regular regional water-quality monitoring plans. Such substances could also serve as tracers to indicate the occurrence of water contamination by accidental spills of FPW.

3.2. Persistence of target compounds

Concerning biodegradability of the target compounds, about 52.5 % of the compounds are readily biodegradable and in one case readily hydrolysable. This observation is consistent with the results in a previous study (Stringfellow et al., 2014), reporting that about 50 % organic hydraulic fracturing chemicals were found biodegradable. Also, Camarillo et al. demonstrated that >30 % of organic chemicals in hydraulic fracturing fluids were biodegradable (Camarillo et al., 2016). This percentage is arguably too low for good environmental stewardship practices. Due to the problematic nature of PMT substances, and persistent substances in general (Cousins et al., 2019), using exclusively readily-biodegradable substances in processes with high potential emissions, like hydraulic fracturing fluids, should be adopted as part of a safe and sustainable design strategy (Hale et al., 2022).
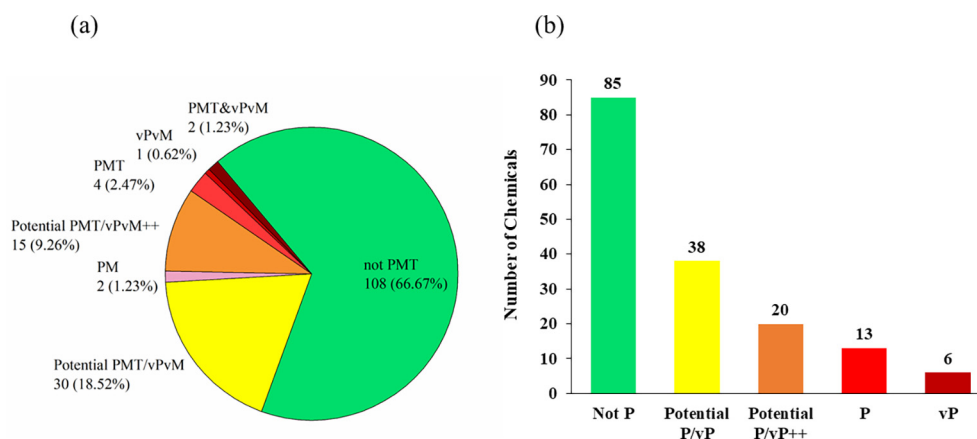
(a)   (b)

Fig. 3. Classification of the target compounds (a) and their persistence (b).
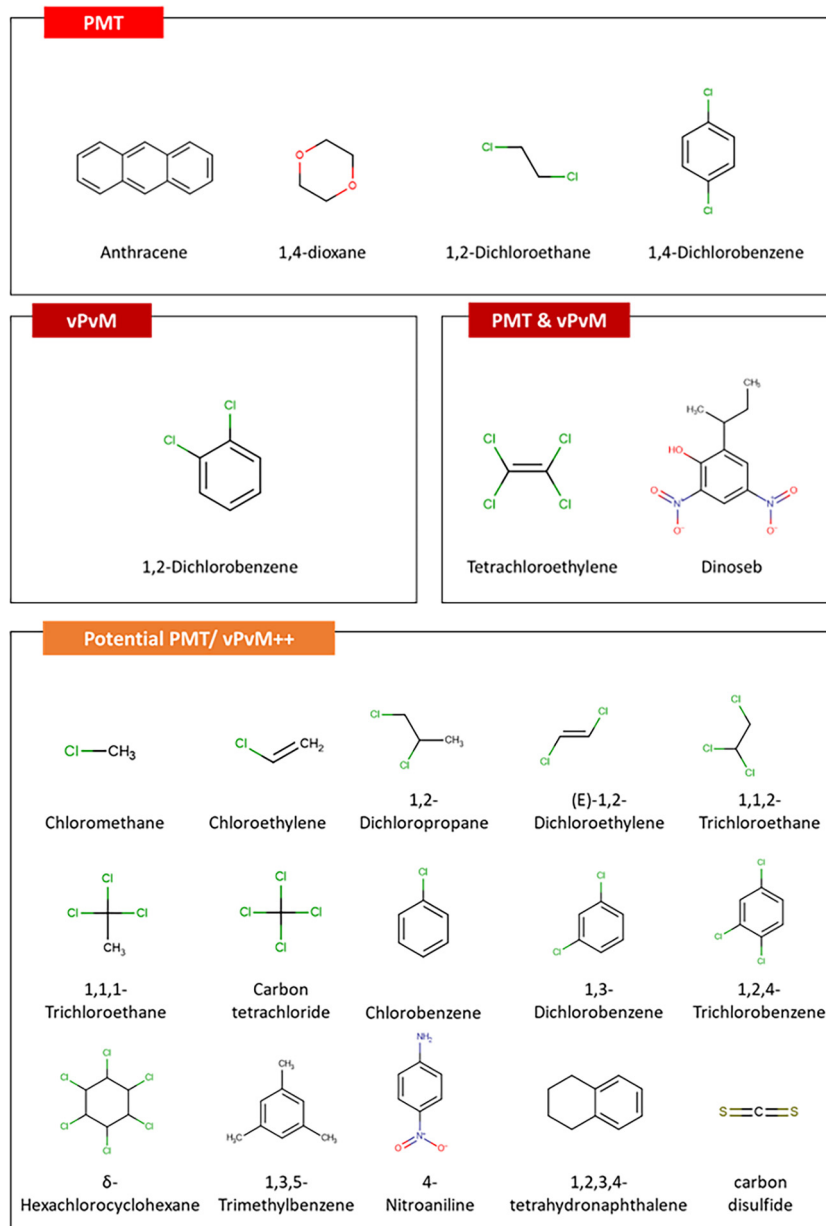
Fig. 4. Molecular structures of substances meeting or strongly suspected to meet the PMT/vPvM criteria based on weight-of-evidence.

3.3. Mobility of target compounds

Concerning the aqueous mobility (M) of the target compounds, 48 substances are identified as "not M". However, the most frequent conclusion for compound mobility assessment is "vM", accounting for 47.5 % of the target compounds. This indicates that these compounds in FPW are mobile in water, and thus could spread faster than "not M" substances in surrounding aquatic environments. This is not unexpected, as the majority of substances produced have a log $K_{oc} < 3$ (though only a small minority of these are also persistent) (Arp and Hale, 2022). That being said, the point of sampling of FPW substances would be to favor the detection of mobile substances, as these are most the likely to return to the surface during hydraulic fracturing and gas production. For instance, a previous study (Rosenblum et al., 2017) observed that about 60–85 % of dissolved organic carbon (DOC) in FPW are hydrophilic. The chemical compositions of FPW vary temporally between formation water and hydraulic fracturing fluids. Specifically, at an early stage of flowback process hydraulic fracturing fluids are dominant, while in the late stage formation water could account for up to 80 % of the composition of the FPW (Yu et al., 2016).

4. Conclusions

Shale gas and oil exploitation is a water-intensive process, producing huge amounts of FPW, and also emissions of PMT/vPvM substances, including the ones identified in this study. Prioritization of the PMT/vPvM substances identified in this study will support risk-based chemical management related to substances used in hydraulic fracturing, such as the establishment of monitoring programs around extraction sites to monitor surrounding water quality. This study is a preliminary investigation that only covers a limited number of the organic compounds that may be present in FPW, where neutral organic compounds were mostly identified by using gas chromatography (GC) based approaches. In recent years, new methods have emerged to better identify and discover highly polar and ionic substances in water media, including liquid chromatography (LC), hydrophilic liquid interaction chromatograph (HILIC), and supercritical fluid chromatography (SFC) based methods coupled with time-of-flight mass spectrometry (TOF-MS) or high resolution mass spectrometry (HRMS) (Neuwald et al., 2021; Oetjen et al., 2017; Schulze et al., 2019b). The chemical characterizations of FPW in future will be facilitated by state-of-art

analytical approaches such as these. Particularly, non-target analytical tools based on HRMS shows a great potential to identify unknown compounds and are increasingly applied to analyze shale gas wastewater (Folkerts et al., 2019; Sun et al., 2019). A special focus for future studies would be to develop efficient sample pretreatment and analytical methods to cover identify a larger range of high-polar ionic substances in FPW, in order to develop a more comprehensive list of PMT/vPvM substances (Koke et al., 2018; Zahn et al., 2020). Moreover, PMT/vPvM-targeted wastewater treatment and remediation strategies will require the development of novel techniques such as foam fractionation (Smith et al., 2022), as well as the integration of currently available and emerging water treatment approaches into novel treatment trains (Hale et al., 2022). Such actions will help minimize long-term impacts on water quality from hydraulic fracturing.

CRediT authorship contribution statement

Chen Huang: Writing - original draft, Investigation, Formal analysis;
Min Han: Investigation, Visualization;
Gan Zhang: Supervision, Validation;
Hans Peter Arp: Methodology, Data Analysis, Writing - review & editing;
Biao Jin: Conceptualization, Writing - original draft, Supervision, Resources.

Data availability

Data used in this report is presented in the Supplementary Data, additional data will be made available on request.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2022.159821.

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