Science of the Total Environment 801 (2021) 149693

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Analysis and prediction of produced water quantity and quality in the Permian Basin using machine learning techniques

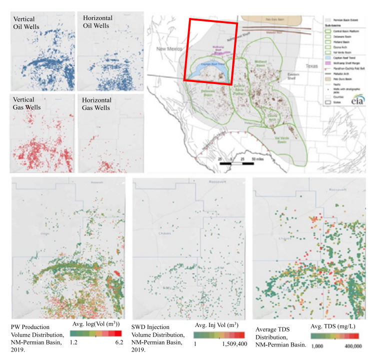
Wenbin Jiang [a], Beepana Pokharel [b], Lu Lin [a], Huiping Cao [b], Kenneth C. Carroll [c], Yanyan Zhang [a], Carlos Galdeano [d], Deepak A. Musale [d], Ganesh L. Ghurye [d], Pei Xu [a,*]

[a] Dept. of Civil Engineering, New Mexico State University, Las Cruces, NM, United States
[b] Dept. of Computer Science, New Mexico State University, Las Cruces, NM, United States
[c] Dept. of Plant and Environmental Science, New Mexico State University, Las Cruces, NM, United States
[d] ExxonMobil Upstream Research Company, Research & Technology Development-Unconventionals, Spring, TX 77389, United States

HIGHLIGHTS

- First study analyzed and predicted PW quantity and quality in the NM-Permian Basin.
- 5-fold cross-validation showed that the RFR model reported high prediction accuracy.
- The ARIMA model showed good results for predicting PW volume in time series.
- Machine learning techniques are useful to PW data analysis and prediction.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 15 June 2021
Received in revised form 11 August 2021
Accepted 11 August 2021
Available online 18 August 2021

Editor: Jay Gan

Keywords:
Produced water quantity
Produced water quality
Produced water reuse
Permian Basin
Statistical analysis
Machine learning

ABSTRACT

Appropriate produced water (PW) management is critical for oil and gas industry. Understanding PW quantity and quality trends for one well or all similar wells in one region would significantly assist operators, regulators, and water treatment/disposal companies in optimizing PW management. In this research, historical PW quantity and quality data in the New Mexico portion (NM) of the Permian Basin from 1995 to 2019 was collected, pre-processed, and analyzed to understand the distribution, trend and characteristics of PW production for potential beneficial use. Various machine learning algorithms were applied to predict PW quantity for different types of oil and gas wells. Both linear and non-linear regression approaches were used to conduct the analysis. The prediction results from five-fold cross-validation showed that the Random Forest Regression model reported high prediction accuracy. The AutoRegressive Integrated Moving Average model showed good results for predicting PW volume in time series. The water quality analysis results showed that the PW samples from the Delaware and Artesia Formations (mostly from conventional wells) had the highest and the lowest average total dissolved solids concentrations of 194,535 mg/L and 100,036 mg/L, respectively. This study is the first research that comprehensively analyzed and predicted PW quantity and quality in the NM-Permian Basin. The results can be used to develop a geospatial metrics analysis or facilitate system modeling to identify the potential opportunities and challenges of PW management alternatives within and outside oil and gas industry. The machine learning techniques developed in this study are generic and can be applied to other basins to predict PW quantity and quality.
© 2021 Elsevier B.V. All rights reserved.

* Corresponding author.
E-mail address: pxu@nmsu.edu (P. Xu).

https://doi.org/10.1016/j.scitotenv.2021.149693
0048-9697/© 2021 Elsevier B.V. All rights reserved.

1. Introduction

Significant volumes of hydraulic fracturing (HF) water and formation water (together known as produced water, PW) are brought to the surface during oil and gas (O&G) exploration and production process (Nicot and Scanlon, 2012). Based on the IHS Markit report, onshore O&G activities in the U.S. would generate nearly 3.18 billion m^3 (20 billion barrels) of PW annually by 2022, reflecting a potential oilfield water market value of $28 billion (Markit I, 2020). Meanwhile, O&G activities require large volumes of water during the drilling and completion process, especially for the development of unconventional resources (Vidic et al., 2013). HF uses large volumes of fracturing fluid (~90% water) to "frack" the low permeable, unconventional plays. It is estimated that water use per well for HF can range from 5700 m^3 to about 60,000 m^3 (1.5 million gallons to 16 million gallons) (USGS, 2021). Water used for HF in the early development of new unconventional O&G wells is usually either reused/recycled produced water and/or locally sourced from surface water or groundwater. The use of fresh water or slightly brackish water for HF may result in local water stress, especially for arid and semiarid areas (Liden et al., 2017).

Unconventional wells usually generate ~3 to 4 times more water than oil (PW to oil ratio, PWOR) compared to PWOR of 13 for conventional wells (Scanlon et al., 2017). However, PW from conventional wells can be reinjected for enhanced oil recovery (EOR), while the PW from unconventional wells needs to be disposed of by other means such as deep well injections (e.g., saltwater disposal wells, SWD wells) or partially treated for HF reuse (Scanlon et al., 2017). Reusing PW reduces local water stress and helps avoid potential environmental concerns. PW reuse has been increasingly implemented inside O&G operations, especially in areas where disposal wells are limited (e.g., Pennsylvania, Ohio, and West Virginia) and where freshwater is scarce (e.g., in parts of West Texas, New Mexico, and California) (Jiménez et al., 2018; Scanlon et al., 2020b).

The Permian Basin is the world's largest unconventional play located in Western Texas and Southeastern New Mexico (Supporting Information, SI, Fig. S1) (Scanlon et al., 2017). Despite the oil crisis in early 2020, oil production in the Permian Basin remained high at 4.3 million barrels (MMbbls) per day, which was more than half of the total onshore U.S. oil production of 7.6 MMbbls per day in February 2021 (U.S. EIA, 2021). The increasing quantity of water used for HF in the Permian Basin has raised concerns about water shortage, especially for New Mexico, which is already facing high water stress (World Resources Institute, 2019). Water issues related to HF may be alleviated by reusing PW for HF of new wells after partial treatment (mostly removal of total suspended solids, oil, iron, and addition of biocide), and it is considered a cost-competitive method in the O&G industry (U.S.EPA, 2020). Scanlon et al. projected that PW volumes exceed HF water demand in the Permian Basin, 1.3 times in the Midland Basin and 3.7 times in the Delaware Basin (Scanlon et al., 2020a). The excess PW has the potential to be beneficially reused outside the O&G field, such as for land application and stream flow augmentation, if it can meet water quality and regulatory requirements after proper treatment. Regulators in New Mexico and Texas are conducting research to understand the environmental, health, and safety risks related to reuse the treated PW for different applications outside of the O&G field.

The reuse of PW in New Mexico could mitigate some water stress and provide economic benefits (Sullivan Graham et al., 2015). Two factors may hinder the beneficial reuse: PW quality and PW quantity. Numerous studies focused on analyzing PW quality and treatment because PW is considered one of the most complex water matrices (Ghurye et al., 2021; Khan et al., 2016; Lin et al., 2020). PW in some areas of the Permian Basin could have high levels of TDS and other geogenic constituents, such as naturally occurring radioactive material (NORM) and hydrocarbons (Chaudhary et al., 2019; Rodriguez et al., 2020). It also contains chemical additives (e.g., acid, biocide, breaker, and surfactant) used during the HF operation (Jiang et al., 2021). More detailed PW composition information can be found in other review papers (Ferrer and Thurman, 2015; Jiang et al., 2021). There have been fewer papers published focused on PW quantity (Cross et al., 2020; Ettehadtavakkol and Jamali, 2019; Scanlon et al., 2020a; Scanlon et al., 2017). Quantifying and forecasting PW volume has great importance to the stakeholders in the O&G industry as well as other water sectors. It helps operators to decide the most suitable methods to handle PW because water disposal costs are typically less than $0.5 per barrel but in some places could go up to $2 per barrel, which could impact well economics (Cross et al., 2020). It could also help regulators to manage the allocation of scarce water resources in that region. Furthermore, it can help the other industries to better coordinate the use of treated PW if used outside the O&G industry. Through better understanding the variability in PW quantity and quality, engineers, industry operators, managers, regulators, and end-users could optimize the design and implementation of PW management methods.

Forecasting PW quantity and quality is challenging due to the large amount of data, and many factors and uncertainties affecting the accuracy of the prediction. Statistical analysis using machine learning techniques is a powerful tool to analyze a large amount of data and make more reliable predictions based on the training data (known data used to optimize the model); and it has been used for PW analysis (Cross et al., 2020; Ettehadtavakkol and Jamali, 2019; Foster et al., 2021).

To the best of our knowledge, there is no published paper that has comprehensively analyzed and predicted PW quantity and quality in the New Mexico portion of the Permian Basin (NM-Permian Basin). This study aims to (1) comprehensively analyze historical and current PW production, disposal, and management situation in the NM-Permian Basin; (2) select appropriate machine learning techniques to predict the PW production profile of different types of oil and gas wells and investigate the attributes affecting production trends; (3) conduct statistical analysis of PW quality in the major formations of the Permian Basin; and (4) identify the knowledge gap and data needs to optimize PW management and beneficial reuse.

2. Materials and methods

2.1. Regression analysis techniques

Regression analysis is the most popular statistical and machine learning technique used to investigate the relationship between a dependent and a set of independent exploratory variables. Both linear and non-linear regression approaches were used in this study. Explanations for linear regression can be found in SI Section S3.1.

2.1.1. Random Forest Regression

The Random Forest Regression (RFR) model is a supervised learning algorithm that uses the ensemble method for prediction. The ensemble method combines the predictions from multiple decision trees to make more accurate predictions than a single model. The decision trees in the RFR model run in parallel. It operates by constructing several decision trees at training time and outputs the result as a mean prediction of the individual trees. The tuning parameters optimized in this study were:

- max_depth: restricts the depth of each tree to prevent overfitting
- n_estimators: controls the number of decision trees in the random forest model. Accuracy usually increases with the number of trees, but the time needed to perform the regression also increases with the number of trees.

The RFR model takes random samples with replacement from the training data set and predicts the output as an average of results of all the decision trees. The idea is that by training each decision tree on different samples, despite each decision tree might have a high variance for a particular set of the training data. Overall, the entire forest will have a lower variance but not at the cost of increasing the bias (Grömping, 2009).

2.1.2. Autoregressive models

A time series is a sequence of measurements of the same variable (s) made over time. An autoregressive (AR) model predicts future behavior based on the past behavior of a variable. It is used for forecasting when there is some correlation between values in a time series and the values that precede and succeed them (Teräsvirta, 1994).

AutoRegressive Integrated Moving Average (ARIMA) model is a type of AR model that uses:

- p: number of autoregressive terms (Autoregressive order)
- d: number of non-seasonal differences needed for stationarity (Differencing order)
- q: number of moving-average terms (Moving Average order)

The ARIMA (p, d, q) model requires data to be stationary, and the Augmented Dickey-Fuller test (ADFuller test) was performed to determine whether the data are stationary. The null and alternate hypotheses of this test are:

- Null Hypothesis: the series has a unit root (The series is non-stationary)
- Alternate Hypothesis: the series has no unit root (The series is stationary)

If the test statistic is less than the critical value, then the null hypothesis is rejected, and the data are considered stationary. The lag(p) for the model was determined based on the Akaike information criterion (AIC), a mathematical method for evaluating how well a model fits the data they were generated from. The model is considered good when the AIC value is low. The value of q is chosen using the Auto Correlation Function (ACF) plot. ACF plot gives the correlation between lagged values of a time series. The ACF plot consists of the correlation values along with the confidence band, and order q is the lag after which ACF crosses the upper confidence interval for the first time.

2.1.3. Evaluation metrics for the regression models

It is crucial to evaluate the performance of the models after their optimization. In other words, it is important to test the ability of the generated models to predict the results based on the training data and testing data.

In this study, coefficient of determination (R^2 score), mean absolute error (MAE), root mean squared error (RMSE), mean absolute percent error (MAPE), and K-fold cross-validation were used to evaluate the optimized models. The Pearson correlation coefficients were used to calculate the correlation between each attribute with the PW production. The explanation for R^2 score, MAE, RMSE, MAPE, and Pearson correlation coefficient can be found in SI Section S3.2.

Cross-validation is a resampling procedure used to evaluate machine learning models to avoid the overfitting issue (Browne, 2000). In a machine learning model, normally, a large percentage (e.g., 70% to 80%) of the data is used as training data and the remaining data are used as the testing data. Because the testing data are randomly selected from the entire data set, the model error varies depending on which part of the data is set as training and testing data. The method with only one train-test split is also referred to as the holdout method. Another method, more commonly used to get robust prediction, is k-fold cross-validation that divides the data set into k subsets and runs the holdout method k times. Every time one of the k subsets is used as the testing set, and the remaining subsets are put together as the training set. Then average error across all k trials is calculated. The advantage of this method is that the model gets to use each data point as the training and testing instance, and the variance in errors is reduced. The disadvantage of this method is that the model needs to run k times resulting in a corresponding increase in computation time.

2.1.4. Software

In this research, Python 3.6.1 was used as the programming language; Jupyter Notebook 5.0.0 was used as the interactive computational environment; scientific libraries used include Numpy 1.19.2, Pandas 1.1.2, Matplotlib 3.3.2, sklearn 0.20.1, scipy 1.5.2, statsmodels 0.12.0. Tableau desktop 2020.3. was used for the geographic information system (GIS) mapping.

2.2. Permian Basin produced water quantity data

The PW quantity data were collected from the New Mexico Oil Conservation Division (NMOCD) FTP server (NMOCD, 2020). In March 2020, the “OCD Interface v1.1” folder had the production data up to January 2020 and was chosen for this research. It had 15 different types of XML files in two subfolders. The detailed XML file information is listed in SI Table S1. The XML files were converted to CSV files using a High-Performance Computing Cluster (Discovery) before performing any pre-processing techniques. The detailed information for each CSV file is in the Supplementary Data “OCD Interface v1.1 Data Dictionary.xlsx”.

2.3. Permian Basin produced water quantity data pre-processing

To identify each unique well in the Permian Basin and facilitate further data analysis, an API (American Petroleum Institute) well number was generated for each well by combining “API state code”, “API county code”, and “API well identifier”, which were provided in the original data files. Then this well API number was added into “wchistory.csv”, “wellhistory.csv”, “wcproduction.csv”, and “wcinjection.csv” files as “WELL_API_NUMBER” attribute.

The core production data were extracted by combining the “wcproduction.csv” and “wellhistory.csv” files. The total number of wells in the NM-Permian Basin (81,444) was determined by adding wells in the four counties in New Mexico: Chaves (7478), Eddy (33,077), Lea (39,113), and Roosevelt (1776). Among these wells, 34,375 were active, and 47,069 were inactive in terms of production. Based on the “directional_status” column, there were 44,874 vertical wells, 11,060 horizontal wells, and 1070 directional wells (there were some wells without directional status information). In this study, for simplification, horizontal wells were considered unconventional, and vertical wells were considered conventional (Scanlon et al., 2017). For the horizontal wells, 329 were drilled before 2010, and 10,731 were drilled after 2010, which reflected the rapid unconventional O&G development in the Permian Basin.

For further analysis, the data were cleaned by deleting invalid data. Invalid data were defined as follows: (1) when any of the targeted attributes of a well equal to 0, such as latitude, longitude, oil production amount, gas production amount, and water production amount; and (2) when the water to oil ratio does not fall into the range of 1 to 100 for oil wells; and when the water to gas ratio larger than 2 (barrels/thousand cubic feet) for gas wells.

RFR models are less sensitive (thus more robust) to the existence of outliers/noise compared with most other machine learning methods because it is an ensemble of decision trees. ARIMA is more affected by outliers than RFR models. Despite these, we are aware that no machine learning method is completely outlier robust. To alleviate the destructive effect of outliers, a widely utilized and accepted strategy is to pre-process data before applying any machine learning techniques. That is why we pre-processed the quantity data to reduce the bad data and possible outliers as discussed above. The outliers were discarded during the cleaning process. There were 402,963 rows of data after year of

1995. After pre-processing the PW quantity data, 311,067 rows of data were used for modeling and projection.

2.4. Permian Basin produced water quality data

PW quality data were downloaded from the United States Geological Survey (USGS) website (USGS, 2020) and extracted from the 'USGSPWDBv2.3n.csv' file. There were 8046 samples available for the NM-Permian Basin. There were 190 columns for each sample to describe the chemical components, sample date, formation, and other attributes. The range of sample dates was from '1929-04-13' to '2001-12-24'. Thus, these data were mostly from conventional wells. The original data used the secondary formation to categorize samples. To investigate the variability of PW quantity and quality between the major formations, samples from the primary formations of Bone Spring, Wolfcamp, Delaware, Artesia, Yeso, and San Andres, were compiled for statistical analysis. In total, there were 3840 samples within these formations with the well API information. Because the PW quality data did not include sufficient data for analysis, data from the Permian Basin Texas side was added into the data set. Also, more recent quality data were extracted from literature (Khan et al., 2016; Nicot et al., 2020; Rodriguez et al., 2020). The quality data were cleaned by applying the following criteria: (1) the TDS concentration falls in the range of 10,000 mg/L to 400,000 mg/L, (2) the concentration of magnesium is lower than the concentration of calcium, (3) pH falls in the range of 2 to 10, and (4) the concentration of calcium, sodium, and chloride are higher than 500 mg/L, 3000 mg/L, and 3000 mg/L, respectively. The quality attributes chosen for analysis were TDS, pH, bicarbonate (HCO_3^-), bromide (Br^-), calcium (Ca^{2+}), chloride (Cl^-), magnesium (Mg^{2+}), potassium (K^+), sodium (Na^+), and sulfate (SO_4^{2-}). After data cleaning, 1919 samples were used for quality analysis.

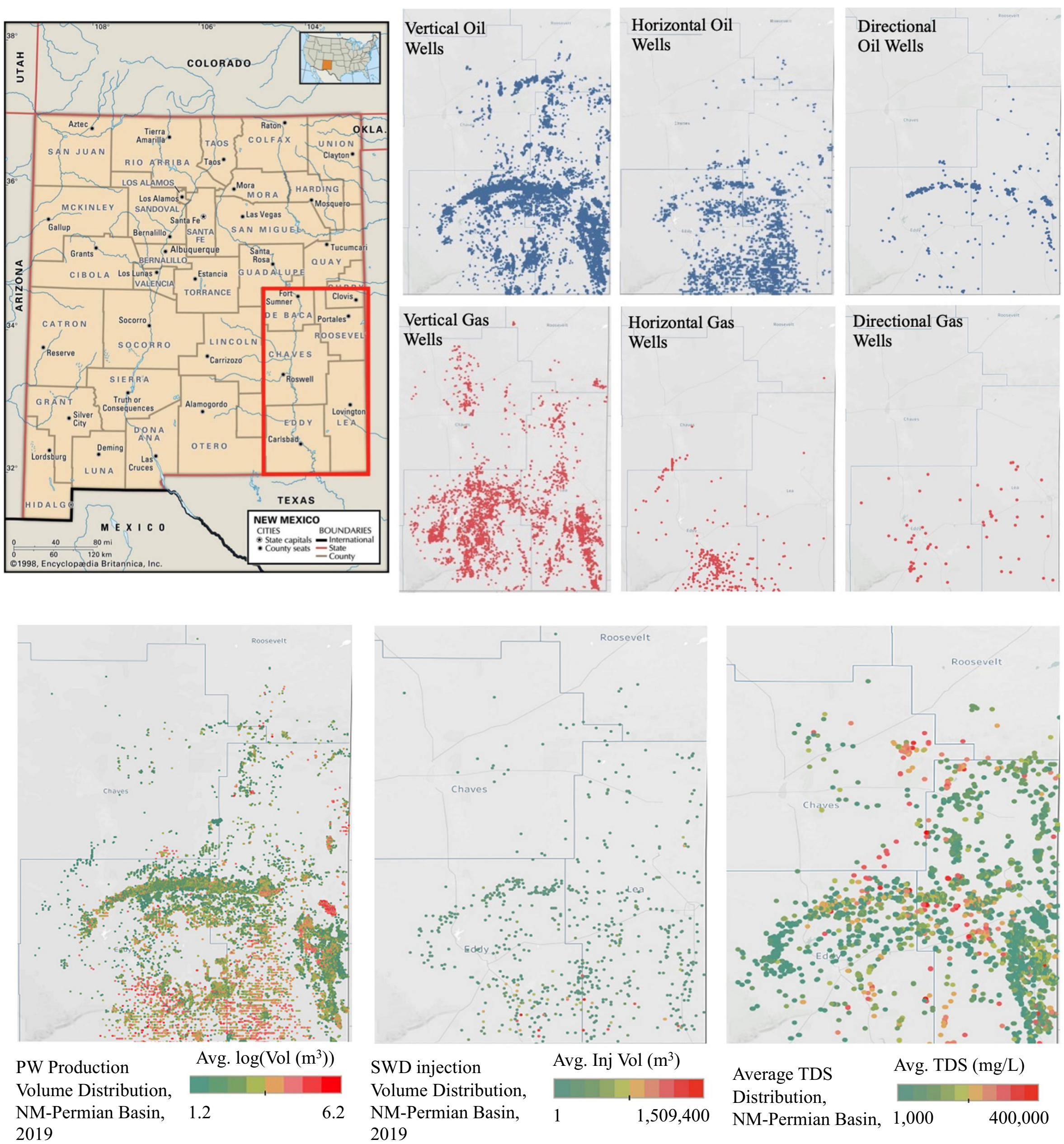


Fig. 1. Different types of wells, produced water (PW) volume in 2019, saltwater disposal (SWD) wells injection volume in 2019, and average PW total dissolved solids (TDS) distribution in the NM-Permian Basin, the red rectangle is the boundary for all graphs. For the PW volume distribution graph, the unit is log10 (Volume (m^3)). NM county map source: (mapofus, 2021).

3. Results and discussion

3.1. Produced water production and management in the NM-Permian Basin

3.1.1. Overview of wells and produced water distribution in the NM-Permian Basin

Fig. 1 shows different types of wells, PW volume from different wells in 2019, saltwater disposal (SWD) wells injection volume in 2019, and average TDS of PW distribution in the NM-Permian Basin. The O&G wells in the NM-Permian Basin are mainly located in Lea, Eddy, Chaves, and Roosevelt counties, as shown in the red rectangle of the NM county map. Horizontal wells are mainly located in the south of Lea and Eddy counties. The maps of well distribution and PW volume distribution show that horizontal (unconventional) wells generate more PW per well than vertical (conventional) wells. This observation is further discussed in Section 3.1.3. PW volumes from horizontal wells and vertical wells are shown in Fig. S2. The SWD injection volume distribution map shows that the SWD wells are widely spread in the region, and their related formations are discussed in Section 3.1.4. Because the PW quality data set lacks samples from unconventional wells, there are fewer data points for the average TDS distribution graphs. PW quality is discussed in Section 3.3. Full-sized graphs are shown in Fig. S3.

3.1.2. PW volume from oil and gas wells, vertical and horizontal wells in the NM-Permian Basin

Fig. 2 shows the change of total PW volume and well numbers for (a) oil wells and (b) gas wells from 1995 to 2019 in the NM-Permian Basin. The data in this graph were not pre-processed, which means some of the wells have missing information, and some of these wells were discarded for the following analysis, as discussed in Section 2. The total volume of PW generated from oil and gas wells increased over time and reached 161.6×10^6 and 32.6×10^6 m^3 (1016 and 204.9 MMbbls) in 2019, respectively. The number of oil and gas wells reached 21,907 and 2850 in 2019, respectively.

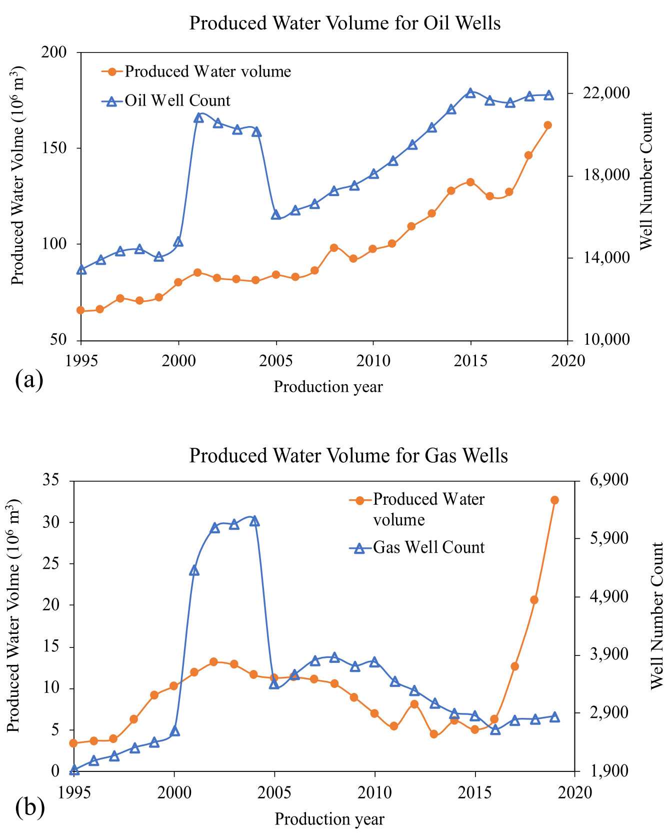


Fig. 2. Produced water volume and well numbers for (a) oil wells and (b) gas wells in the NM-Permian Basin from 1995 to 2019. Supporting Information Fig. S4 has English unit information.

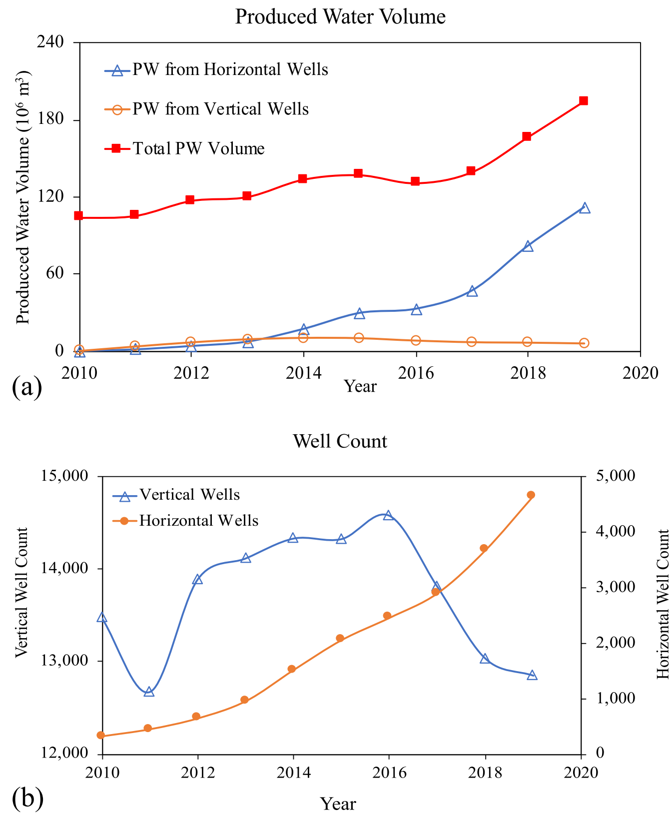


Fig. 3. (a) Total produced water volume, produced water volume from horizontal wells and vertical wells; (b) Well numbers for horizontal wells and vertical wells in the NM-Permian Basin from 2010 to 2019. Supporting Information Fig. S4 has English unit information.

The rapid increase of PW volume from 2010 to 2019 was caused by the unconventional development (Fig. 3a). The difference between the total PW volume data was because (1) the total PW volume was not pre-processed while other data were pre-processed, as discussed in Section 2.2. Data in the following part of this study were all pre-processed; (2) many wells were not reported or reported without well directional information. Well numbers for horizontal wells increased more than 10 times (319 to 4642) from 2010 to 2019 in the NM-Permian Basin; while vertical wells stayed relatively stable around 13,500 (Fig. 3b).

Fig. 4 shows the percentage of PW volume generated from different formations in the NM-Permian Basin in 2019, and detailed data can be found in SI Table S2. Understanding which formations produce most of the PW would help to predict the PW production for developing new O&G wells and to optimize the PW management methods. The formations that generated most of the PW were: Bone Spring (24.9%), San Andres (16.6%), Wolfcamp (14.8%), Purple Sage (Wolfcamp) pool (14.7%), Artesia (9.2%), Yeso (7.8%), and Delaware (5.3%). Among these formations, Purple Sage (Wolfcamp) pool mainly produces gas, and other formations mainly produce oil. The Bone Springs, Wolfcamp, and Delaware (full name: Delaware Mountain Group) formations are where most of the unconventional wells are located (Popova, 2020).

3.1.3. Production profile over operational months for different types of wells

Average oil and gas volume, PW volume, and PW to oil and gas ratio during the well lifetime were calculated for wells in the Permian Basin to investigate their production trend (Figs. 5 and 6). Wells drilled after 2010 were chosen because most of the horizontal wells were drilled after 2010 (Fig. 3b).

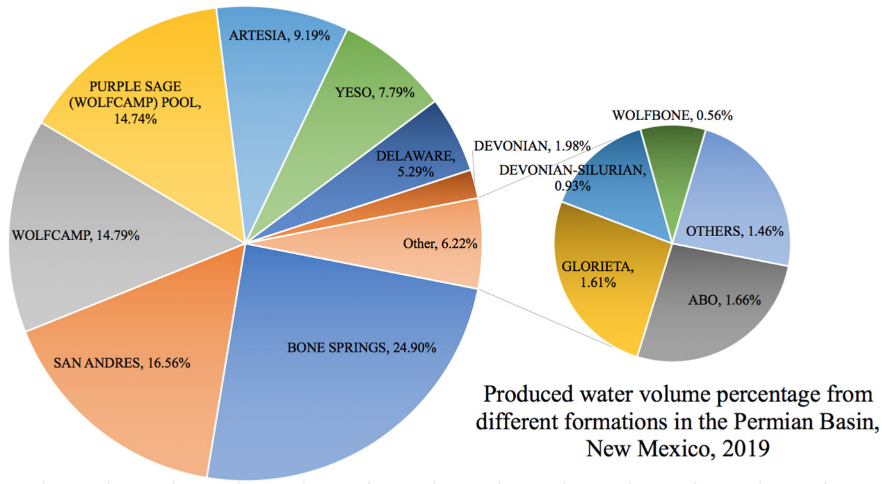


Fig. 4. Produced water volume percentage from different formations in the NM-Permian Basin, 2019. Detailed data can be found in SI Table S2.

For horizontal oil wells, the average PW volume was 19,560 m^3 (0.123 MMbbls) per well in 2019, similar to horizontal oil wells from other basins/formations (e.g., Bakken: 22,740 m^3/well (0.143 MMbbls); Niobrara: 18,440 m^3/well (0.116 MMbbls); Monterey: 28,300 m^3/well (0.178 MMbbls)) (Kondash et al., 2017). For horizontal gas wells, vertical oil wells, and vertical gas wells in the Permian Basin, the average PW volume was 48,330 m^3, 3340 m^3, and 2540 m^3 (0.304, 0.021, and 0.016 MMbbls) per well in 2019. These results proved the observation in Section 3.1.1 that, on average, horizontal wells generated more PW than vertical wells in 2019. However, the average water-to-oil ratio is smaller for horizontal oil wells (3 to 6) than for vertical oil wells (5 to 7), which is consistent with a previous study (Scanlon et al., 2017). For gas wells, the average water to gas ratio is higher (0.2–0.6) for horizontal gas wells compared to vertical gas wells (0.1).

Oil, gas, and PW volume reached the maximum in the first few months then decreased (Figs. 5 and 6). Before 40 months, PW volume declined fast, and then stabilized. For horizontal wells, the initial large volume of PW is mainly the flowback water which is the water injected for HF. In most cases, flowback water has a TDS level close to that of the injected HF fluid, and the TDS increases quickly over time when formation water starts to become the major portion (Jiang et al., 2021; Kondash et al., 2017; Oetjen et al., 2018). Based on previous research, the flowback stage often ends in 1 to 2 months (Kondash et al., 2017; Oetjen et al., 2018). Thus, the peaks in Figs. 5 and 6 are mainly formation water, which has high TDS. SI Fig. S7 shows the average cumulative percentage of PW volume in the total production of wells (120-months

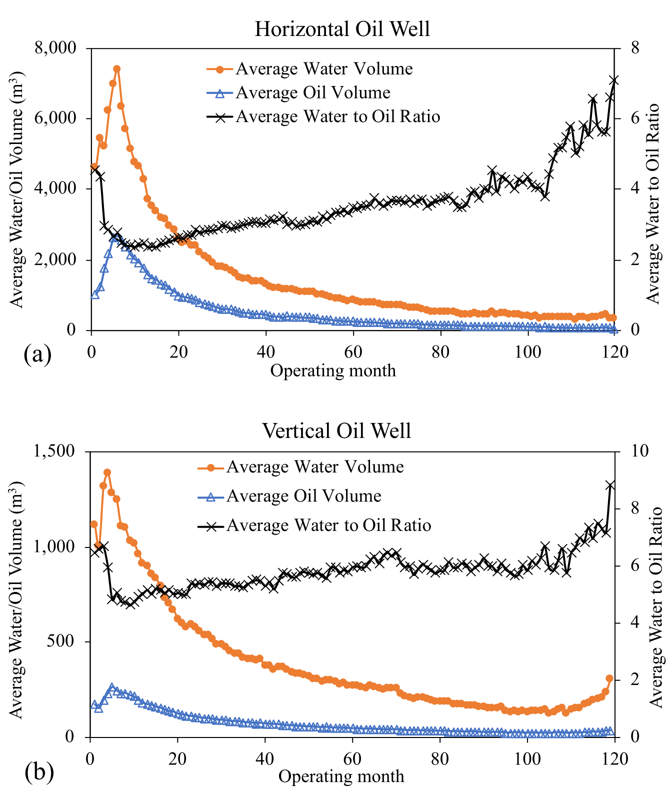


Fig. 5. Average oil production, average produced water production, and average produced water to oil ratio profile for (a) horizontal oil well and (b) vertical oil well drilled after 2010 in the NM-Permian Basin. Fig. S5 has English unit information.

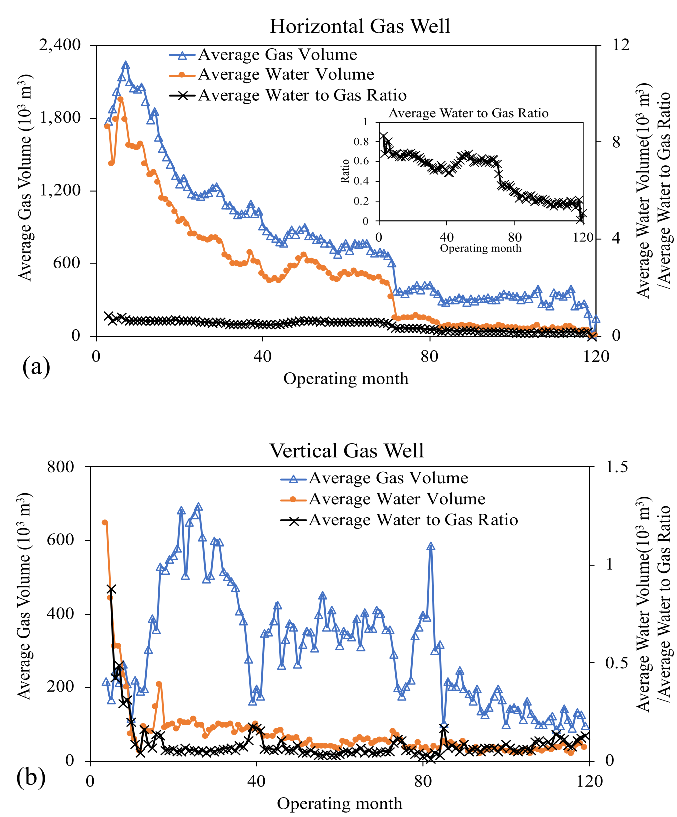


Fig. 6. Average gas production, average produced water production, and produced water to gas ratio profile for (a) horizontal gas well and (b) vertical gas well drilled after 2010 in the NM-Permian Basin. Fig. S6 has English unit information.

from 2010 to 2019). On average, horizontal wells only generate ~6% of total PW volume (flowback water) in the first two months, which agrees with other research that the total PW from horizontal wells is mainly composed of naturally occurring formation water (Birdsell et al., 2015; Gallegos et al., 2015). Horizontal oil wells in the Permian Basin produce ~ 20% and ~ 50% of the total PW in 6 months and 19 months for a 120-month lifetime range, similar to horizontal oil wells in the Bakken and Niobrara Basin (Kondash et al., 2017). The months for vertical oil well, horizontal gas well, and vertical gas well to reach 50% of the total PW volume are 27, 26, and 32, respectively. Thus, the O&G wells produce a large amount of PW in the first two years.

These trends in quantity and quality would be important factors to consider when planning PW reuse. Flowback water with lower TDS (if freshwater or brackish water is used for HF) and relatively larger volume in the early stages of operation could be treated and used for new HF fluid because it usually contains chemical additives, and their impact on the environment outside the O&G field is still under research. After several months, the PW volume decreases and the TDS increases to match formation water salinity, thus the risk associated with chemical additives would be lower because most of the PW is the formation water. The major concern at this stage would be the risks associated with the high salinity, naturally occurring substances, such as petroleum hydrocarbons, NORM, and heavy metals (Jiang et al., 2021; Kondash et al., 2017; Lin et al., 2020). Based on the trends and data observed, it seems logical to consider segregation and separate treatment of flowback water and PW because they may need different treatment for potential reuse; however, such an approach may not be practical and economical to implement in the field.

3.1.4. PW management in the NM-Permian Basin

PW is commonly managed by reusing it in O&G operations (e.g., enhanced oil recovery - EOR, hydraulic fracturing) or disposing it via SWD wells, which could have some induced seismicity concerns (Keranen et al., 2014; Langenbruch and Zoback, 2016). Understanding the PW volumes available for reuse versus disposal would provide context on how much PW volumes could be reduced for disposal and available for beneficial use.

Fig. 7 shows the trend of PW used for EOR and SWD in the Permian Basin since 2010. In 2013, the volume of PW injected into SWD wells exceeded the volume of PW used for EOR mainly due to the increase in unconventional activities. In 2019, the volume of PW injected into SWD and EOR reached 85.9×10^6 m^3 (540 MMbbls) and 46.9×10^6 m^3 (295 MMbbls), respectively. Fig. 8 shows the percentage of PW used for (a) SWD wells and (b) EOR in each formation in the Permian Basin in 2019. Detailed data are in SI Table S3 and S4. From Fig. 8, the Devonian Formation received 46.8% of PW injected into the SWD wells, and the San Andres Formation received 53.9% of the PW used for EOR.

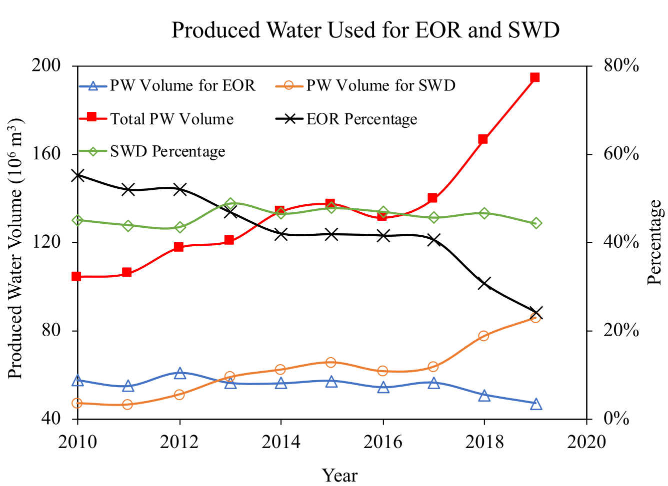


Fig. 7. Produced water volume used for enhanced oil recovery (EOR) and saltwater disposal (SWD) well injection in the NM-Permian Basin from 2010 to 2019. Fig. S8 has English unit information.

3.2. Analysis using machine learning techniques

3.2.1. Correlation between attributes and PW volume

The correlation between each attribute and the PW volume is measured by calculating the Pearson correlation coefficient. Linear regression and RFR models were also applied to each attribute. MAE and R^2 scores were calculated to evaluate the performance of each model. The regression models used in this process have each attribute value as the input and PW volume as the output. Tables 1 and 2 present the results for horizontal oil well and horizontal gas well analyses, respectively. For the horizontal oil wells, the Pearson correlation coefficient (-Section S3.1) shows a strong correlation between oil production amount (0.73), years of operation (−0.27), and measured vertical depth (0.23) with PW volume. These results mean the PW volume has a positive correlation with the oil production amount and the measured vertical depth but has a negative correlation with the years of operation. In the RFR model, the oil production amount has the highest R^2 score of 0.6, greater than the R^2 score (0.53) from the linear regression model. Similar results were observed for the horizontal gas well, PW volume has a high Pearson correlation coefficient with the gas production amount (0.82), measured vertical depth (0.36), gas price (−0.36), and years of operation (−0.33). In the RFR model, the gas production amount has the highest R^2 score of 0.74, which was greater than the R^2 score (0.66) from the linear regression model. These results suggested the RFR model would be a better method to predict the PW volume than the linear regression model. Thus, the RFR model was used for the following analysis to predict PW volume based on several attributes simultaneously.

3.2.2. Random Forest Regression models with K-fold cross-validation

In this section, all the attributes, including well latitude and longitude, true vertical depth, measured vertical depth, year of operation, county, formation, and oil or gas production amount, were chosen as the RFR model input simultaneously to evaluate their relationship with PW volume. During the analysis, the data set was divided into a training set (80%) and a testing set (20%). When the regression is performed on the partitioned data, the scores are specific to the training and testing instances, and the model may give different scores for other partitions. To prepare a model that uses all the instances in both the training and testing step, the cross-validation method is used. K-fold cross-validation ($k = 5$) method is used to predict the PW volume to reduce the variance in errors, and the score is the average of the five runs. After optimization, parameters for the RFR model were set as following: n_estimators = 50, max_depth = 23, n_splits = 5.

Table 3 shows the average R^2 score and MAE of the RFR model with 5-fold cross-validation for different types of wells in the Permian Basin. The vertical wells have higher instances number compares to other types of wells. Overall, the RFR model has high R^2 scores (> 0.8) for all types of wells except the directional gas well (0.70). The reason for this exception is the low instance number (566). Machine Learning models usually require a large number of data points to achieve high performance. Thus, the RFR model showed a good ability to predict PW volume based on the selected attributes. With the development of the O&G industry in the Permian basin, more data points will be collected in the future, which will increase the model's accuracy and reliability.

3.2.3. Time series analysis: autoregressive models

For the RFR model, PW volume is predicted by other attributes of the well related to PW production. For the time series analysis, the objective is to predict PW volume at a certain date/time based on the previous

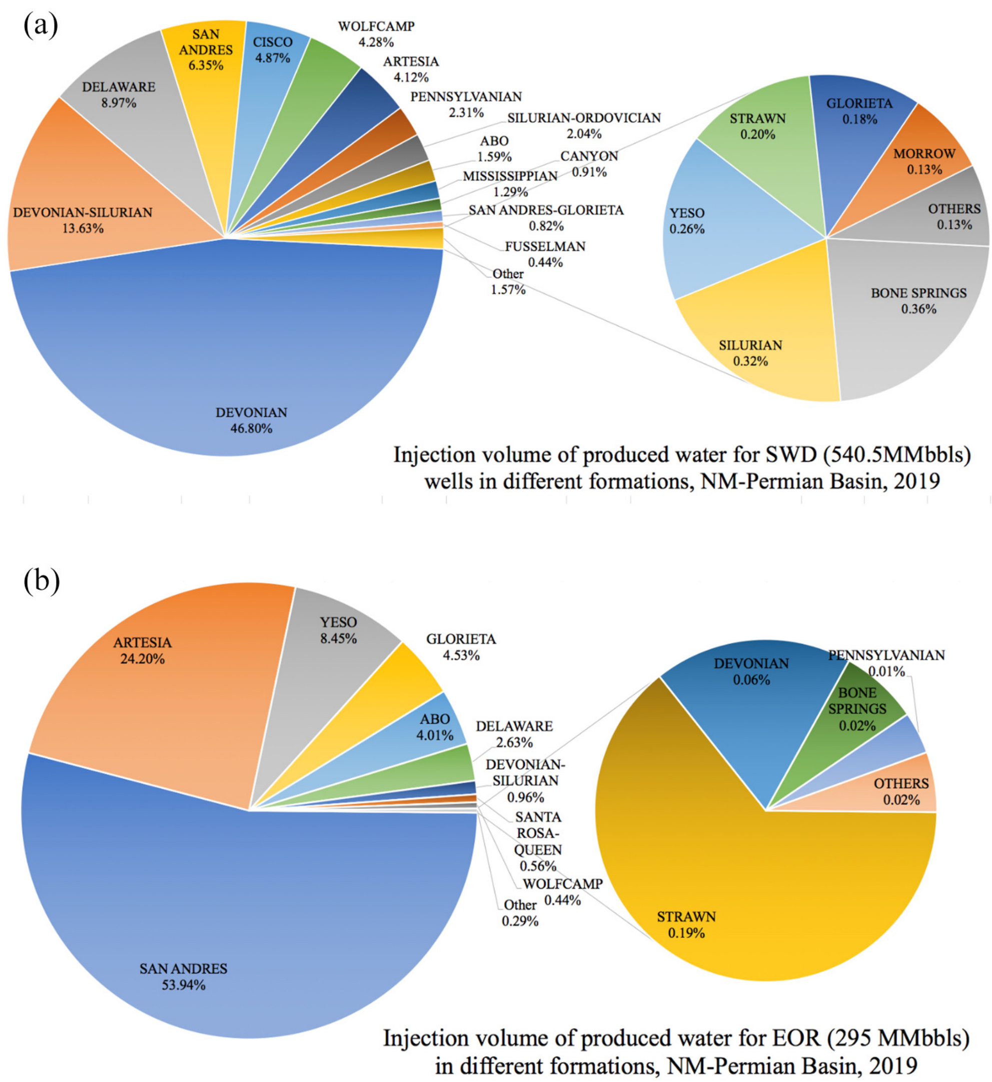


Fig. 8. Produced water volume for (a) saltwater disposal (SWD) well injection and (b) enhanced oil recovery (EOR) in different formations in the NM-Permian Basin, 2019.

production data. The data used for this model are the monthly average PW volume per well in Bone Springs and Wolfcamp Formations because these are the two important unconventional formations in the Permian Basin (Section 3.1.2). The time series model used in this study is the ARIMA (p, d, q) model. "p" is the number of time lags (months in this study) that the next prediction depended on. For example, if $p = 2$,

Table 1
Mean Absolute Error (MAE) and Coefficient of Determination (R^2 scores) for predicting produced water volume in horizontal oil wells using one attribute at a time, and Pearson Correlation Coefficient for each attribute with produced water volume.

Attributes	Random Forest Regression		Linear regression		Pearson correlation coefficient
	MAE	R^2 score	MAE	R^2 score	
prod_amt_oil	45,804	0.60	55,249	0.53	0.73
oil_price	89,898	0.011	90,639	0.0011	−0.04
dpth_tvd_num	64,099	0.37	90,042	0.011	0.12
dpth_mvd_num	60,442	0.44	87,608	0.06	0.23
latitude	57,511	0.50	88,796	0.025	−0.17
longitude	60,050	0.46	90,614	−0.00028	0.035
latitude and longitude	53,310	0.54	88,719	0.025	NA
formation_numeric	81,143	0.14	88,962	0.030	0.18
Years_of_operation	81,547	0.11	85,611	0.079	−0.27
county	90,493	0.0025	90,702	−0.0008	0.021

Note: prod_amt_oil: amount of oil production; dpth_tvd_num: true vertical depth; dpth_mvd_num: measure vertical depth; NA: not available.

Table 2
Mean Absolute Error (MAE) and Coefficient of Determination (R^2 scores) for predicting produced water volume in horizontal gas wells using one attribute at a time, and Pearson Correlation Coefficient for each attribute with produced water volume.

Attributes	Random Forest Regression		Linear regression		Pearson correlation coefficient
	MAE	R^2 score	MAE	R^2 score	
prod_amt_gas	45,623	0.74	571,57	0.66	0.82
gas_price	103,306	0.22	119,391	0.13	−0.36
dpth_tvd_num	63,729	0.47	126,148	0.034	0.17
dpth_mvd_num	64,278	0.42	114,056	0.19	0.36
latitude	57,131	0.54	104,512	0.19	−0.40
longitude	60,275	0.47	121,673	0.043	0.20
latitude and longitude	56,966	0.53	104,062	0.20	NA
formation_numeric	117,371	0.04	125,199	0.027	0.16
Years_of_operation	106,575	0.15	117,237	0.095	−0.33
county	110,342	0.12	125,798	0.012	0.16

Note: prod_amt_gas: amount of gas production; dpth_tvd_num: true vertical depth; dpth_mvd_num: measure vertical depth; NA: not available.

Table 3
Mean Absolute Error (MAE) and Coefficient of Determination (R^2 score) of RFR Model using 5-fold Cross-Validation for different types of wells in the NM-Permian Basin.

Data set	Number of instances	R^2 score	MAE
Vertical oil well	229,506	0.87	6016
Horizontal oil well	20,738	0.87	23,460
Directional oil well	4372	0.83	16,402
Vertical gas well	24,891	0.86	3816
Horizontal gas well	2167	0.91	24,107
Directional gas well	566	0.70	3412

the previous two months data are modeled to predict next month's production. “d” is the number of non-seasonal differences; it is used to make the time series stationary because the ARIMA model requires the time series data whose mean/variance do not change over time. The other term “q” is the moving average which is the lag after ACF crosses the upper confidence interval for the first time in the ACF plot. In this study, only 0 lays above the confidence interval, so $q = 0$ was used.

After calculation and optimization, ARIMA (6, 1, 0) model and ARIMA (4, 1, 0) model were chosen for the Bone Springs and Wolfcamp Formations, respectively. Then the models were fitted to the training data to predict the PW volume for the next month. After the predicted data were recorded, the true production volume for that month was added to the training data to make the subsequent prediction. Continuously updating the training data with each month's true average PW amount assists in getting the best prediction for the next month. Fig. 9 shows the true average PW volume per well and the predicted average PW volume per well in the (a) Bone Springs and (b) Wolfcamp Formations each month from 2018 to 2019. RMSE, MAE, and MAPE were calculated for these two predictions to evaluate the performance of the models (Fig. 8). The MAPE for the Bone Springs Formation and Wolfcamp Formation is 5.4% and 5.6%, respectively. Also, the models have low RMSE and MAE scores. These results suggest the ARIMA model is an excellent candidate to predict PW volume for the time series analysis when proper parameters are chosen.

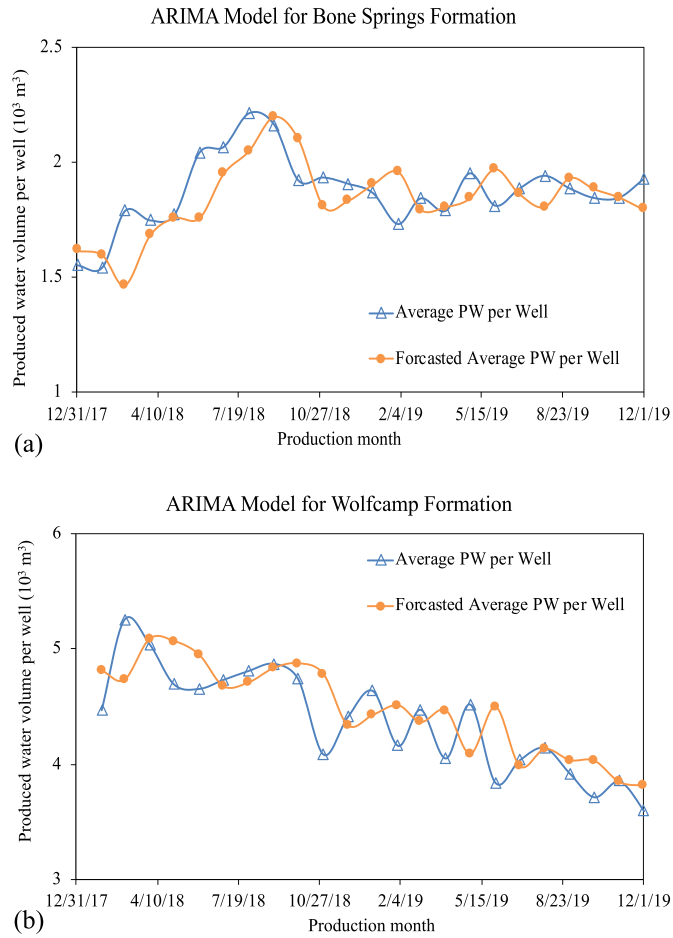


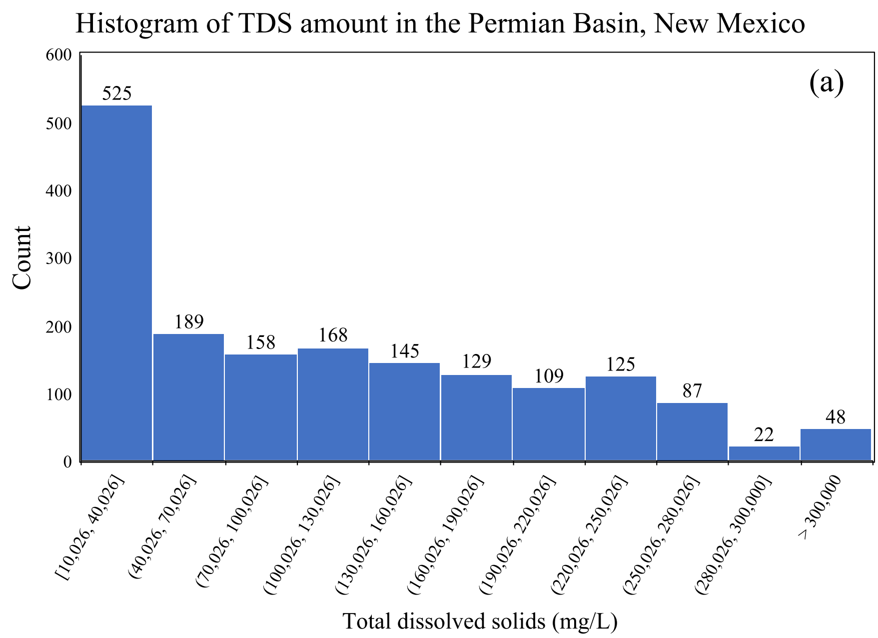
Fig. 9. AutoRegressive Integrated Moving Average (ARIMA) model for horizontal oil wells in (a) Bone Spring Formation (ARIMA (6, 1,0)) and (b) Wolfcamp Formation (ARIMA (4, 1,0)). The root mean square error (RMSE, unit: barrels per well), mean absolute error (MAE, unit: barrels per well), and mean absolute percent error (MAPE) for Bone Spring Formation are 834, 645, and 5.4%. The RMSE, MAE, and MAPE for Wolfcamp Formation are 1937, 1492, and 5.6%. Fig. S9 has English unit information.

3.3. Statistical analysis for produced water quality in the Permian Basin

Analysis and characterization of PW quality in geospatial distribution and formation is critical to choose proper treatment based on its quality and reuse applications. Fig. 1 shows the geospatial distribution of TDS levels for PW across the NM-Permian Basin. Fig. 10a shows the distribution of TDS levels from the consolidated PW samples in the NM-Permian Basin. From these samples, ~ 30% have TDS lower than 40,000 mg/L and ~ 60% have TDS lower than 100,000 mg/L. Fig. 10b shows the distribution of TDS levels from the consolidated PW samples in the whole Permian Basin, ~ 20% have TDS lower than 40,000 mg/L, and ~ 55% have TDS lower than 100,000 mg/L. However, the ranges for TDS and histogram distributions are similar for both, 113,706 $\pm$ 89,573 mg/L (total sample counts 1706) for the NM-Permian and 115,401 $\pm$ 83,926 mg/L (total sample counts 3879) for the whole Permian Basin (NM + TX), which suggests that there are no significant differences in the statistics for these two sets of data.

Table 4 shows statistical summary (minimum, maximum, and mean) of PW quality (TDS, pH, Mg^{2+}, Ca^{2+}, Cl^-, Na^+, K^+, SO_4^{2-}, Br^-, and HCO_3^-) in the whole Permian Basin and six major formations (San Andres, Artesia, Bone Springs, Yeso, Wolfcamp, and Delaware). It shows that the PW samples from the Delaware Formation has the highest average TDS (194,535 mg/L), and the PW samples from the Artesia Formation has the lowest average TDS (100,036 mg/L). Even though these have significant differences in average TDS, the Artesia Formation (or Group of Formations) and the Delaware Mountain Formation (or Group of Formations) are both parts of the Guadalupian-age evaporite cap-rock that trapped a significant amount of the oil and gas, and these are where much of the oil and water production has occurred. Chaudhary et al. found that multiple processes including evaporite dissolution and seawater evaporation contributed to the brine evolution for waters of the Delaware and the Artesia seemed to show more of an influence of evaporite dissolution (Chaudhary et al., 2019). However, Engle et al. noted that sulfate reduction has also impacted the brine geochemistry of both of these Formations/Groups (Engle et al., 2016). The combination of brine evolution processes and variability in fluid flow within both the Artesia Formation and the Delaware Mountain Formation make it uncertain to determine the reasons for difference in TDS statistics between these formations. This illustrates the need and potential for using machine learning techniques for further quantifying impacts of multiple processes in the tectonic, sedimentary and hydrogeological contexts.

Understanding the distribution of PW quality from different formations could assist in selecting and developing appropriate fit-for-purpose treatment technologies. For example, for hydraulic fracturing, suspended solids, oil, and iron in PW need to be removed by settling, chemical precipitation, coagulation and flotation. For low salinity PW (<30,000–45,000 mg/L TDS), reverse osmosis (RO) can be used for salts removal (Chang et al., 2019), however, the high concentration of Ca^{2+} and TOC may cause membrane fouling and require extensive pretreatment. Techniques such as thermal distillation, membrane distillation, and solar still can be used to treat PW with high salinity (Chen et al., 2021; Wang et al., 2019). Depending on the constituents in PW,



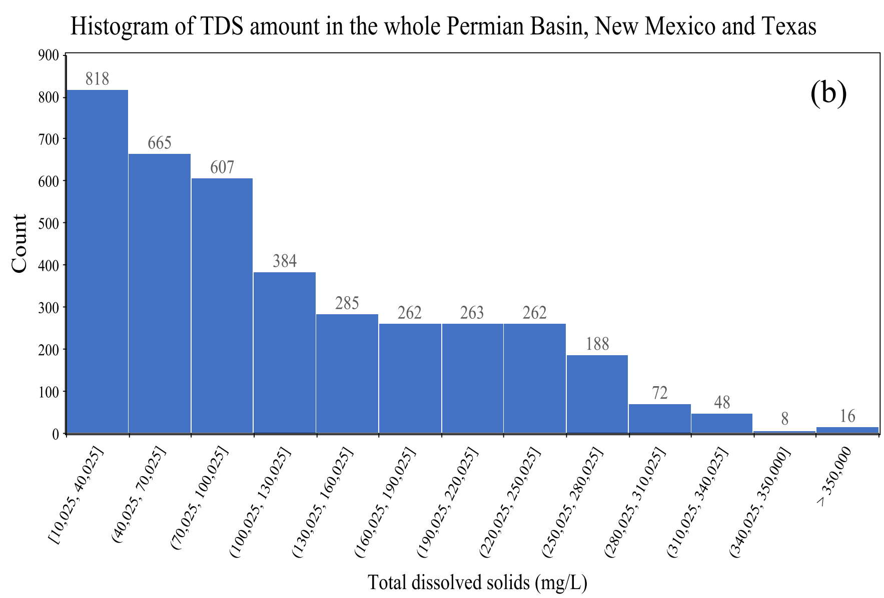


Fig. 10. Histogram, based on available PW samples, of TDS levels in the (a) NM-Permian Basin; (b) Permian Basin including New Mexico and Texas.

valuable chemicals may be recovered such as salts, struvite, calcite, and gypsum (Hu et al., 2021; Hu et al., 2020).

The limitation of the PW quality data in this study is that most of the PW samples were from conventional wells before 2001. More samples from unconventional wells in recent years need to be collected and analyzed in the future to better understand the PW quality distribution in the Permian Basin.

4. Conclusion and future work

In a first-of-its-kind study, historical PW quantity and quality data in the NM-Permian Basin were collected, pre-processed, and analyzed by statistical methods and machine learning techniques. The primary conclusions of this study are listed below.

- In 2019, the total PW volume generated in the NM-Permian Basin from oil and gas wells reached 161.6×10^6 and 32.6×10^6 m^3 (1016 and 204.9 MMbbls), respectively. The formations that generated most of the PW in 2019 were Bone Spring (24.9%), San Andres (16.6%), Wolfcamp (14.8%), Purple Sage (14.7%), Artesia (9.2%), Yeso (7.8%), and Delaware (5.3%).
- The historical PW quantity analysis shows that horizontal oil wells in the NM-Permian Basin produced more PW per well than vertical wells despite lower PWOR. The average PW volume for horizontal oil wells was 19,560 m^3 (0.123 MMbbls) per well in 2019. Horizontal oil wells in the Permian Basin produce ~20% and ~ 50% of the total PW in 6 months and 19 months for a 120-month lifetime range. The months for vertical oil well, horizontal gas well, and vertical gas well to reach 50% of the total PW volume are 27, 26, and 32, respectively.
- In 2019, the PW volume injected into SWD and EOR reached 85.9×10^6 m^3 (540 MMbbls) and 46.9×10^6 m^3 (295 MMbbls) in the NM-Permian Basin, respectively. The Devonian Formation received 46.8% of PW injected into the SWD wells, and the San Andres Formation received 53.9% of the PW used for EOR.
- For the horizontal oil wells, the Pearson correlation coefficient shows a strong correlation between oil production amount (0.73), years of

Table 4
Statistical summary of produced water quality (min-max/mean values) for the whole Permian Basin and six major formations.

	Permian Basin	Wolfcamp Formation	Delaware Formation	Artesia Formation	Yeso Formation	Bone Spring Formation	San Andres Formation
TDS (mg/L)	11,265-391,007/ 125,679	12,972-297,557/ 118,064	22,174-360,545/ 194,535	11,265-384,963/ 100,036	16,342-381,108/ 112,105	24,841-255,451/ 167,119	11,345-391,007/ 127,968
pH	2.1–9.9/6.9	2.8–9.4/6.8	3.7–8.9/6.8	4.2–9.9/7.3	4.7–8.8/6.8	6.3–7.1/6.8	2.1–9.2/6.9
Ca (mg/L)	522–60,073/ 6903	572–46,500/ 5432	640–46,346/ 12,759	522–25,315/ 2827	685–28,913/ 4463	1260-21,720/ 9735	530–60,073/ 8234
Na (mg/L)	3030-143,085/ 38,275	3310-102,000/ 38,249	5253-119,990/ 56,805	3030-133,343/ 34,089	3315-107,396/ 37,209	7600-80,469/ 52,268	3067-143,085/ 36,978
K (mg/L)	24–45,680/ 1000	60–1410/ 470	99–45,680/ 1296	24–4620/ 498	41–1570/ 466	724–1232/ 978	59–33,962/ 1746
Mg (mg/L)	2.2–24,800/ 1961	15–12,211/ 1183	98–8246/ 2566	55–18,400/ 1305	2.2–8544/ 1430	170–3397/ 1571	2.7–24,800/ 2369
Cl (mg/L)	3159-241,303/ 75,164	4635-186,000/ 70,026	12,600-225,613/ 117,183	3159-222,596/ 59,169	6600-237,245/ 67,710	13,177-156,699/ 84,880	4010-241,303/ 76,811
Sulfate (mg/L)	3.1–11,553/ 2305	3.1–10,800/ 1933	25–7522/ 1294	19–11,553/ 3071	287–5957/ 2378	500–2350/ 1011	45–8881/ 2230
Br (mg/L)	3–1519/426	10–1050/524	186–1519/618	3–528/139	240–276/252	NA	22–517/184
HCO3 (mg/L)	3–5131/ 541	5–1850/ 530	3–1266/ 201	18–5131/ 687	5–1520/ 539	189–891/ 416	7–3860/ 538
TOC (mg/L)	53–184/123	NA	NA	NA	NA	NA	NA

Note:
Data format: min-max/mean.
TOC: Total Organic Carbon.
NA: not available.

operation (−0.27), and measured vertical depth (0.23) with PW volume. After optimization, parameters for the RFR model were set as: n_estimators = 50, max_depth = 23, n_splits = 5. Overall, the RFR model with five-fold cross-validation has high R^2 scores (> 0.8) for all types of wells except the directional gas well (0.70). The ARIMA (6, 1, 0) and ARIMA (4, 1, 0) models for the Bone Springs Formation and Wolfcamp Formation gave good predictions for the PW volume in the time series analysis.
- From the PW quality analysis, around 20% of the PW samples have TDS levels lower than 40,000 mg/L in the Permian Basin. PW samples from the Delaware Formation has an average TDS of 194,535 mg/L, whereas PW samples from the Artesia Formation has an average TDS of 100,036 mg/L. In this study, most of the PW samples used for quality analysis were from conventional wells. There were limited PW quality data from unconventional wells in the Permian Basin to conduct a machine learning analysis.

The results from this study would facilitate the O&G industry to evaluate future PW production and optimize PW management accordingly, such as identifying the potential locations to treat PW and the locations that treated PW could be used for other applications, which are under investigation by the authors. Currently, the online PW data are either not analyzed for easy use or require a high subscription fee for access. The authors are preparing a database for free public access to the analyzed data and used methods in this study. It is expected that with the development of unconventional resources, more samples will be collected for different basins. Machine learning techniques tested in this work with quantitative data could be applied to conduct PW data analysis in the future. Also, the machine learning techniques used in this study can be applied to other areas to predict the quantity and quality of PW or other products of interest. In this study, the PW quality data are mostly from conventional wells and with limited water quality parameters (e.g., TDS and major ions). For beneficial use of PW, there is an urgent need to conduct comprehensive water quality analysis of conventional as well as unconventional PW including inorganic and organic matter, NORMs, and toxicity.

CRediT authorship contribution statement

B. Pokharel, W. Jiang, L. Lin, H. Cao, P. Xu for data analysis, programing, and modeling; W. Jiang and B. Pokharel for writing the original draft and editing; H. Cao, K.C. Carroll, Y. Zhang, C. Galdeano, D.A. Musale, G.L. Ghurye, and P. Xu for research design and implementation, and editing the manuscript; C. Galdeano and P. Xu for managing the research project.

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.

Acknowledgments

The authors thank the ExxonMobil Upstream Research Company, New Mexico Produced Water Research Consortium, and New Mexico Water Resources Research Institute for financial and technical support.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2021.149693.

References

Birdsell, D.T., Rajaram, H., Lackey, G., 2015. Imbibition of hydraulic fracturing fluids into partially saturated shale. Water Resour. Res. 51, 6787–6796.
Browne, M.W., 2000. Cross-validation methods. J. Math. Psychol. 44, 108–132.
Chang, H., Li, T., Liu, B., Vidic, R.D., Elimelech, M., Crittenden, J.C., 2019. Potential and implemented membrane-based technologies for the treatment and reuse of flowback and produced water from shale gas and oil plays: a review. Desalination 455, 34–57.
Chaudhary, B.K., Sabie, R., Engle, M.A., Xu, P., Willman, S., Carroll, K.C., 2019. Spatial variability of produced-water quality and alternative-source water analysis applied to the Permian Basin, USA. Hydrogeol. J. 27, 2889–2905.
Chen, L., Xu, P., Kota, K., Kuravi, S., Wang, H., 2021. Solar distillation of highly saline produced water using low-cost and high-performance carbon black and airlaid paper-based evaporator (CAPER). Chemosphere 269, 129372.
Cross, T., Sathaye, K., Darnell, K., Niederhut, D., Crifasi, K., 2020. Predicting Water Production in the Williston Basin Using a Machine Learning Model. Unconventional Resources Technology Conference, 20–22 July 2020. Unconventional Resources Technology Conference (URTeC), pp. 3492–3503.
Engle, M.A., Reyes, F.R., Varonka, M.S., Orem, W.H., Ma, L., Ianno, A.J., et al., 2016. Geochemistry of formation waters from the wolfcamp and "Cline" shales: insights into brine origin, reservoir connectivity, and fluid flow in the Permian Basin, USA. Chem. Geol. 425, 76–92.
Ettehadtavakkol, A., Jamali, A., 2019. A data analytic workflow to forecast produced water from Marcellus shale. J. Nat. Gas Sci. Eng. 61, 293–302.
Ferrer, I., Thurman, E.M., 2015. Chemical constituents and analytical approaches for hydraulic fracturing waters. Trends Environ. Anal. Chem. 5, 18–25.
Foster, J., Misra, S., Osogba, O., Bhatia, M., 2021. Machine learning assisted detection of excess water-producing wells in unconventional shale plays. J. Nat. Gas Sci. Eng. 104025.

Gallegos, T.J., Varela, B.A., Haines, S.S., Engle, M.A., 2015. Hydraulic fracturing water use variability in the U nited S tates and potential environmental implications. Water Resour. Res. 51, 5839–5845.

Ghurye, G.L., Mishra, D., Lucas, L., 2021. Thermal desalination of produced water—an analysis of the partitioning of constituents into product streams and its implications for beneficial use outside the O&G industry. Water 13, 1068.

Grömping, U., 2009. Variable importance assessment in regression: linear regression versus random forest. Am. Stat. 63, 308–319.

Hu, L., Yu, J., Luo, H., Wang, H., Xu, P., Zhang, Y., 2020. Simultaneous recovery of ammonium, potassium and magnesium from produced water by struvite precipitation. Chem. Eng. J. 382, 123001.

Hu, L., Wang, H., Xu, P., Zhang, Y., 2021. Biomineralization of hypersaline produced water using microbially induced calcite precipitation. Water Res. 190, 116753.

Jiang, W., Lin, L., Xu, X., Cheng, X., Zhang, Y., Hall, R., et al., 2021. A critical review of analytical methods for comprehensive characterization of produced water. Water 13, 183.

Jiménez, S., Micó, M., Arnaldos, M., Medina, F., Contreras, S., 2018. State of the art of produced water treatment. Chemosphere 192, 186–208.

Keranen, K.M., Weingarten, M., Abers, G.A., Bekins, B.A., Ge, S., 2014. Sharp increase in central Oklahoma seismicity since 2008 induced by massive wastewater injection. Science 345, 448–451.

Khan, N.A., Engle, M., Dungan, B., Holguin, F.O., Xu, P., Carroll, K.C., 2016. Volatile-organic molecular characterization of shale-oil produced water from the Permian Basin. Chemosphere 148, 126–136.

Kondash, A.J., Albright, E., Vengosh, A., 2017. Quantity of flowback and produced waters from unconventional oil and gas exploration. Sci. Total Environ. 574, 314–321.

Langenbruch, C., Zoback, M.D., 2016. How will induced seismicity in Oklahoma respond to decreased saltwater injection rates? Sci. Adv. 2, e1601542.

Liden, T., Clark, B.G., Hildenbrand, Z.L., Schug, K.A., 2017. Unconventional oil and gas production: waste management and the water cycle. Advances in Chemical Pollution, Environmental Management and Protection. 1. Elsevier, pp. 17–45.

Lin, L., Jiang, W., Chen, L., Xu, P., Wang, H., 2020. Treatment of Produced Water with Photocatalysis: Recent Advances, Affecting Factors and Future Research Prospects. Catalysts 10, 924.

mapofus, 2021. NM County Map.

Markit I, 2020. Produced Water from Onshore US Oil and Gas Activities to Decline to Nearly 20 Billion Barrels Annually; Reach $28 Billion in Value by 2022, IHS Markit Says 2021. IHS Markit.

Nicot, J.-P., Scanlon, B.R., 2012. Water use for shale-gas production in Texas, US. Environ. Sci. Technol. 46, 3580–3586.

Nicot, J.-P., Darvari, R., Eichhubl, P., Scanlon, B.R., Elliott, B.A., Bryndzia, L.T., et al., 2020. Origin of low salinity, high volume produced waters in the Wolfcamp Shale (Permian), Delaware Basin, USA. Appl. Geochem. 122, 104771.

NMOCD, 2020. New Mexico Produced Water Quantity Data (ftp://164.64.106.6/Public/OCD/).

Oetjen, K., Chan, K.E., Gulmark, K., Christensen, J.H., Blotevogel, J., Borch, T., et al., 2018. Temporal characterization and statistical analysis of flowback and produced waters and their potential for reuse. Sci. Total Environ. 619, 654–664.

Popova, O., 2020. Permian Basin, Part 1, Wolfcamp, Bone Spring, Delaware Shale Plays of the Delaware Basin, Geology Review. U.S. Energy Information Administration.

Rodriguez, A.Z., Wang, H., Hu, L., Zhang, Y., Xu, P., 2020. Treatment of produced water in the permian basin for hydraulic fracturing: Comparison of different coagulation processes and innovative filter media. Water 12, 770.

Scanlon, B.R., Reedy, R.C., Male, F., Walsh, M., 2017. Water issues related to transitioning from conventional to unconventional oil production in the Permian Basin. Environ. Sci. Technol. 51, 10903–10912.

Scanlon, B.R., Ikonnikova, S., Yang, Q., Reedy, R.C., 2020a. Will water issues constrain oil and gas production in the United States? Environ. Sci. Technol. 54, 3510–3519.

Scanlon, B.R., Reedy, R.C., Xu, P., Engle, M., Nicot, J., Yoxtheimer, D., et al., 2020b. Can we beneficially reuse produced water from oil and gas extraction in the US? Sci. Total Environ. 717, 137085.

Sullivan Graham, E.J., Jakle, A.C., Martin, F.D., 2015. Reuse of oil and gas produced water in south-eastern New Mexico: resource assessment, treatment processes, and policy. Water Int. 40, 809–823.

Teräsvirta, T., 1994. Specification, estimation, and evaluation of smooth transition autoregressive models. J. Am. Stat. Assoc. 89, 208–218.

U.S.EIA, 2021. Drilling Productivity Report. U.S. Energy Information Administration, U.S.E.I.A.

U.S.EPA, 2020. Summary of Input on Oil and Gas Extraction Wastewater Management Practices Under the Clean Water Act Final Report. U.S.EPA.

USGS, 2020. U.S. Geological Survey National Produced Waters Geochemical Database v2.3.

USGS, 2021. How much water does the typical hydraulically fractured well require? https://www.usgs.gov/faqs/how-much-water-does-typical-hydraulically-fractured-well-require?qt-news_science_products=3#qt-news_science_products (2021)

Vidic, R.D., Brantley, S.L., Vandenbossche, J.M., Yoxtheimer, D., Abad, J.D., 2013. Impact of shale gas development on regional water quality. Science 340.

Wang, H., Lu, L., Chen, X., Bian, Y., Ren, Z.J., 2019. Geochemical and microbial characterizations of flowback and produced water in three shale oil and gas plays in the central and western United States. Water Res. 164, 114942.

World Resources Institute, 2019. Aqueduct 3.0 Country Rankings. World Resources Institute.