A Multivariate Outlier Detection Approach for Water Footprint Assessments in Shale Formations: Case Eagle Ford Play (Texas)

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Abstract: The increasing trend on water use for hydraulic fracturing (HF) in multiple plays across the U.S. has raised the need to improve the HF water management model. Such approaches require good quality datasets, particularly in water stressed regions. In this work, we presented a QA/QC framework for HF data using a multivariate outlier detection methodology based on five univariate techniques: two interquartile ranges at 95 and 90% (PCTL95, PCTL90), the median absolute deviation (MAD) and Z-score with thresholds of two and three times the standard deviation (2STD, 3STD). The "cleaning" techniques were tested using two data sources centered on the Eagle Ford play (EFP), Texas, for the period 2011-2017. Results suggest that the multivariate PCTL95 and MAD techniques are the best choices to remove long-tailed statistical distributions, classifying the minimum number of records as outliers. Overall, outliers represent 13-23% of the total HF water volume in the EFP. In addition, outliers highly impacted minimum and maximum HF water use values (min-max range of 0-47 m^3/m and 5.3-24.6 m^3/m of frac length, before and after the outlier removal process, respectively), that are frequently used as a proxy to develop future water-energy scenarios in early-stage plays. The data and framework presented here can be extended to other plays to improve water footprint estimates with similar conditions.

Keywords: Outliers; Geospatial Analysis; Water Use; Hydraulic Fracturing; Eagle Ford, Shale Gas.

INTRODUCTION

Quantifying water use for hydraulic fracturing (HF) has becoming a key issue related to water security in many regions where shale (or tight rock) based energy are located, because shale development has been perceived as a water-intensive practice (Pacsi et al., 2014; Scanlon et al., 2014; Scanlon et al., 2017; Walker et al., 2017). HF and horizontal drilling techniques have been used to increase oil and gas production from U.S. shale formations during the last decade, contributing to the country's energy independence (Lin et al., 2018; Nicot and Scanlon, 2012). Nevertheless, production from unconventional reservoirs using HF has been related to several environmental issues, such as soil degradation and habitat losses (Slonecker et al., 2012; Pierre et al., 2015; Thompson et al., 2015), surface water and groundwater contamination by wastewater discharge or splits (Vidic et al., 2013; Warner et al., 2013; Vengosh et al., 2014; Schwartz, 2015), and seismic events induced by produced water injection and disposal (Frohlich, 2012; Atkinson et al., 2016; Hennings et al., 2019).

HF impacts on water resources are mainly associated with baseflow reduction in rivers (Barth-Naftilan et al., 2015; Sharma et al., 2015; Arciniega-Esparza et al., 2017), local groundwater depletion (Scanlon et al., 2014; USEPA, 2015) and conflicts with other water users at a temporal scale (Horner et al., 2016; Scanlon et al., 2017; Walker et al., 2017).

Overall, negative effects of HF development are highly variable spatially and depend on many factors, such as geology, economy, location, climate, operators' experience, well attributes and stimulation steps, among others (Nicot and Scanlon, 2012; Gallegos et al., 2015; Gallegos and Varela, 2015; Ikonnikova et al., 2017; Walker et al., 2017). The literature reported HF water volumes that range from ~1,000 to 70,000 m^3 per well across U.S. (Kondash and Vengosh, 2015; Kondash et al., 2018), where unconventional drilling with horizontal laterals tend to require much more water than unconventional vertical wells and conventional wells (Goodwin et al., 2013).

The increasing trend of water intensity during HF operations over the last years in multiple plays across U.S. has led some to suggest the need HF water management models (Ikonnikova et al., 2017; Walker et al., 2017; Kondash et al., 2018). In previous studies, methodologies based on historical records of HF water use were applied to assess future water demands, hydrocarbon production and wastewater disposal (Nicot and Scanlon, 2012; Pacsi et al., 2014; Horner et al., 2016; Ikonnikova et al., 2017). Nevertheless, in undeveloped plays around the world, the lack of local data forces users toward data and statistics from active plays as a proxy to further evaluate potential water impacts from newer plays (Guo et al., 2016; Yu et al., 2016; Galdeano et al., 2017; Hernández-Espriú et al., 2019; Williamson and Esterhuyse, 2019).

Because models to generate scenarios are data dependent, good quality data and longer records are required to improve projections. However, examples of data cleaning processes (data mining), which comprise the identification of anomalous values (outliers) and patterns in water-related HF datasets, are scarce in the current literature. Univariate outlier detection methods are frequently applied to quality assure HF water databases. Boxplot or inter quartile range have been the most common methodologies to identify suspicious data (Goodwin et al., 2013; Oikonomou et al., 2016; Kondash et al., 2018; Hernández-Espriú et al., 2019), followed by standard deviation-based methods (Walker et al., 2017). Furthermore, several studies that analyzed multiple plays did not specify how they treated outliers (Nicot and Scanlon, 2012; Gallegos et al., 2015; Kondash and Vengosh, 2015; Chen and Carter, 2016; Horner et al., 2016).

In this study, a comparative outlier detection approach is presented. We integrated two databases (FracFocus and IHS) to assess HF water consumption across the Eagle Ford play, located in central Texas, USA. A multivariate outlier detection technique is proposed from univariate statistical schemes using well attributes that are related to water consumption. The following five multivariate outlier detection methodologies were applied: (1) an interquartile range using a threshold at 95% (PCTL95), (2) interquartile range at 90% (PCTL90), (3) the median absolute deviation method

(MAD), (4) Z-score using 3 times the standard deviation (std) as threshold (3STD) and (5) Z-score using 2 times std as threshold (2STD).

This study differs from prior works because here we report the outlier-related statistics and compare the effects of removing outliers within the HF water footprint. In addition, we compute the space-time evolution of unconventional development in terms of water use, proppant load, lateral length, vertical depth, and well density from the two databases, to explore the differences between FracFocus and IHS, in both county and play-wide levels.

Thus, the objectives of our work are to: (1) compare multivariate techniques for outlier detection on HF datasets to improve HF water use estimates, (2) evaluate the differences between FracFocus and IHS databases related to HF water use, (3) evaluate the influence of several well attributes on HF water use, (4) update the space-time evolution of HF development within the Eagle Ford play with variables that are frequently used to propose HF scenarios in emergent plays, and (5) provide a reproducible framework to be applied in other plays, worldwide.

STUDY AREA

The Eagle Ford play

The study area comprises the Eagle Ford shale play, in Texas (Fig 1a), a transboundary shale formation between south-central Texas and northeast Mexico that covers a U.S. area of ~46,500 km^2 (~6.8% of the area of Texas) and intersects 27 counties with a total population of ~1.2 million inhabitants (in 2016). A total of ~55% of its entire population is distributed across three major counties: Webb, Brazos and Guadalupe.

[Insert Fig 1 here]

The regional climate varies from temperate at the northeast with an aridity index (potential evaporation/precipitation) of 1.4, to a semiarid climate with an aridity index of 3 (Trabucco and Zomer, 2009). Annual precipitation ranges from 1,050 mm/year to 480 mm/year. The landscape is predominantly flat with an average slope of 1.5° and a mean elevation of 157 m.a.s.l. The land cover is dominated by shrubs (45%), followed by grass (20.4%), cultivated crops (6.5%), deciduous forest (5.5%) and urban areas (4%) (derived from Homer et al., 2015).

Groundwater pumping across the play reached 585.7 Mm^3 in 2016 (TWDB, 2018), dominated by irrigation (321.8 Mm^3, 55%), municipal (177.1 Mm^3, 30.2%) and mining (41.6 Mm^3, 7.1%), with 54% of total water abstractions concentrated in Brazos, Frio, Gonzalez and Robertson counties.

The main groundwater sources include the regional aquifers of Carrizo-Wilcox (throughout), Gulf Coast (at the south) and Edwards (at the north). The Carrizo-Wilcox aquifer overlaps about 80% of the play extent and represents an important water source for municipal and irrigation water uses (~50.5% of total water use is withdrawn from the Carrizo-Wilcox aquifer, TWDB, 2018). Furthermore, it is an important source of brackish water for HF in the region (Nicot and Scanlon, 2012).

The play extent is crossed by nine major rivers that generally flow southeast and discharge toward the Gulf of Mexico, including Rio Grande and Nueces River at the south, and the Colorado River and Brazos River at the north. Several rivers receive significant contributions from aquifers during dry periods (Green et al., 2008; Arciniega-Esparza et al., 2017). Although surface water withdrawals in Texas are restricted in many regions due to allocations and low availability, withdrawals for HF activities from the main reach of Rio Grande have been reported in adjacent counties (Scanlon et al., 2014).

HF activities in Eagle Ford play

The Eagle Ford play is one of the largest oil and gas producers (see production zones in Fig 1b) in the U.S., with a long history of horizontal wells drilling using HF techniques (Nicot and Scanlon, 2012; Scanlon et al., 2014). Unconventional development at the Eagle Ford started in 2008 in La Salle county. Land alteration from oil and gas activities, mainly due to pipeline construction, during the last decade has been documented (Pierre et al., 2015).

Maximum intensity of HF activities were reported during 2014 with more than 4,000 horizontal wells drilled, demanding ~95 Mm^3 of water (Ikonnikova et al., 2017). Such volume represented ~16 % of total groundwater pumpage in Texas for 2016, nevertheless, a small fraction of HF water volume is composed by flowback and recycled water, and 60-80% is composed by brackish water from deep formations that did not impact the domestic water demands (Scanlon et al., 2014). A total of 14,500 HF wells were drilled from 2010-2016 and this number is expected to raise from 20,000 to 87,000 new wells over the next 25 years, depending on market conditions (Scanlon et al., 2014; Ikonnikova et al., 2017).

Despite the high rates of HF water requirements, direct impacts to water sources have not been reported, nor any conflicts with stakeholders during drought events, such as the exceptional drought that occurred during 2011-2012 (Scanlon et al., 2013, 2014; Arciniega-Esparza et al., 2017).

MATERIALS AND METHODS

Datasets

Our data mining is based on the following two databases: FracFocus Chemical Disclosure Registry version 3.0 (https://fracfocus.org/), a website that provides an open database managed by the Ground Water Protection Council and the Interstate Oil and Gas Compact Commission. FracFocus delivers information on hydraulic fracturing, mainly focused on chemicals, searchable on the API number (a 10-digit unique code that identifies each well), beginning and end of fracturing operations, operator's name, drilling depth (or total vertical depth, TVD), total base water volume (HF water use), and total base no water volume (volume of hydraulic fluid that is not water, TBnW). FracFocus started operating in 2011 and is updated monthly (around the 15th day). The database currently includes information from 23 states, with more than 80,000 disclosures recorded by more than 1,000 companies. FracFocus database is available in a Microsoft SQL structure and as comma separated values file (csv) from http://fracfocusdata.org/digitaldownload/fracfocuscsv.zip.

The second dataset used is IHS Enerdeq (IHS Energy, 2011), a private database complementary to FracFocus that contains well construction properties such as well direction, horizontal length, total vertical depth, producing formation, stimulation method, fracturing stages, proppant volume and detailed information about the drilling process, among other things. Unlike FracFocus, IHS distinguishes the type of water quality (fresh, slick and saltwater).

FracFocus and IHS wells across the Eagle Ford play are shown in Fig 1c and Fig 1d, respectively. The analysis period was chosen from 2011 to 2017, as few wells were found in FracFocus database prior to 2011. In this study, FracFocus is considered as the main dataset since it can be used for reproducible research. Nevertheless, IHS information is required for a more thorough analysis.

Software

We used open-source tools for data processing. Data mining and statistical analysis of the two databases were performed using Python 3.6 (Python Software Foundation, 2013), a cross-platform, object-orient programming and dynamic typing language that has been used recently for data science, deep learning, and data mining. Some of the most widely used Python packages include: Pandas (McKinney and Team, 2015), a data analysis tool for simple data structures such as time series and numerical tables; SciPy (Oliphant, 2007), Python's standard library for scientific computing that contains a set of statistical tools; Scikit-learn (Pedregosa et al., 2011), a straightforward and efficient data mining and machine-learning toolkit; Statsmodels (Seabold and Perktold, 2010), a set of statistical models aimed at data testing and exploration; and Seaborn

(Waskom, 2018), a powerful visualization library that displays state-of-the-art and informative charts and graphs.

The geospatial analysis component was generated on SAGA GIS V. 6.4 (Conrad et al., 2015), an open-source and cross-platform geographic information system (GIS) that provides several algorithms for geoscientific analysis. Nevertheless, some spatial analysis was computed in QGIS 3.2 Bonn (QGIS Development Team, 2015), which is probably one of the most popular open-source GIS platforms and that is comparable with ArcGIS (ESRI, 2013) in many geoscience applications.

Statistical methods

Statistical analyses were focused on HF water use and other variables that influence the water use intensity in a well. For the purposes of this study, seven variables from FracFocus and 13 from IHS were used. Full description and label of the variables used are shown in Table 1. For IHS dataset, HF water volume was considered as the sum of three water volumes from different sources (water, slick water and saltwater) to be comparable with FracFocus total base water volume (TBW), while other fluid volumes for HF were summed as TBnW (Total Base no Water Volume).

[Insert Table 1 here]

Outlier Detection and Assessment

A data quality control (QC) procedure was conducted to detect missing values and suspicious data in both datasets. An initial quality filter consisted of removing records when total base water volume (TBW), initial and final HF activities dates (JobStartDate and JobStartEnd) were absent (see attributes description at Table 1). Wells with zero values on true vertical depth (TVD) were removed, as well as other evident outliers, such as TBW > 150,000 m^3, TVD > 10,000 m and number of days required for hydraulic stages (FracJob) > 90 days.

We tested three univariate statistical strategies for outlier detection, including the interquartile range (IQR) method, the median absolute deviation (MAD) method and the Z-score method (standard deviation). The IQR method defines that an outlier occurs when one of the conditions in Eq. 1 is true:

$$\begin{aligned} x_i &< X_{25} - d\,IQR \\ x_i &> X_{75} + d\,IQR \end{aligned} \qquad (1)$$

where X_{25} is the lower quartile (25%), X_{75} is the upper quartile (75%), IQR is the interquartile range defined as X_{75}–X_{25}, and *d* is another factor with an assumed value of 3 for detecting extreme outliers or 1.5 to define mild outliers (Barbato et al., 2011). The IQR method is poor sensitive to alterations due to outliers and it does not consider sample size. Nevertheless, for large datasets, this method tends to remove genuine values (Barbato et al., 2011). In this study, the IQR method was tested considering d as 3 and 1.5.

The MAD method is considered a robust measure of scale of a data sample as it is less affected by outliers than the standard deviation. MAD is computed as the median of all absolute deviations from the median (Huber, 1981), as shown in Eq. 2:

$$MAD = b\, M_i\left(\left|x_i - M_j\left(x_j\right)\right|\right) \qquad (2)$$

where M_i is the median of the series and *b* usually is 1.4826, linked to assumption of normality (Rousseeuw and Hubert, 2011; Leys et al., 2013). Outlier detection with this criteria is achieved with the equation proposed by Leys et al. (2013) and Miller (1991):

$$|x_i - M| > 3\, MAD \qquad (3)$$

where *M* is the median and *MAD* is the mean absolute deviation (Eq. 3). Nonetheless, in spite of the robustness of MAD, it seems that the Z-score is more efficient for data that follows a normal distribution (Rousseeuw and Hubert, 2011).

The Z-score uses a normal (Gaussian) distribution and assumes that outliers occur when the absolute value of observed data minus its mean value is larger than the standard deviation, multiplied by a factor commonly between 2 or 3, as following:

$$|x_i - \bar{x}| \geq c\,\sigma \qquad (4)$$

where x_i is the current value, $\bar{x}$ the mean value, σ the standard deviation and c is either 3 for detecting extreme outliers that occur only 0.13 % of all cases (Howell, 1998), or 2 for detecting mild outliers (Miller, 1991). One disadvantage of this methodology are the assumptions of a normal distribution and that $\bar{x}$ and σ are altered by outliers (Leys et al., 2013). In this study, 3σ and 2σ were tested to identify outliers.

Consider the use of two values for each d (Eq. (1)) and c (Eq. (4)), five multivariate outlier detection techniques were applied. Since the proposed methodologies are used to detect outliers for single variables, multivariate outlier detection was carried out following the methodology suggested by Zhao (2012), where a record is assumed to be an outlier if one or more attributes are detected as outliers using the univariate method.

Statistical Analysis

A statistical analysis was carried out using several steps. First, correlations and regressions between variables in each database were determined. Temporal evolution was then carried out to analyze trends for future projections. In the case of IHS dataset, additional variables were computed and analyzed, such as the water use intensity with respect to the lateral length and proppant load. Subsequently, a comparison between FracFocus and IHS databases was done only for common variables, such as TBW and TVD.

On the other hand, wells from IHS were classified as conventional vertical, conventional horizontal, unconventional vertical and unconventional horizontal (Scanlon et al., 2017), to determine the water footprint between different technologies. Water footprint classification depend on TBW, lateral length, and proppant load (Table S1); thus, an appropriate classification using the FracFocus database was not possible. Borehole horizontal length and TVD from IHS were recomputed through a 3D well borehole reconstruction using the "down-hole survey" data (see full description in Fig S1) to distinguish between true and false horizontal wells, following the criteria proposed in Scanlon et al. (2017).

Parametric and non-parametric statistical tests (T-test, Mann-Whitney, One-Way ANOVA, Kruskal-Wallis) were applied to test significance of differences on HF water use and related well attributes between well technologies, production zones, and temporal evolution.

Geostatistical Analysis

Spatial analysis was carried out to assess the evolution of oil and gas development in terms of (1) HF water use, (2) well density, and (3) area required for the hydrocarbon production. HF water use was compared between oil and gas production zones (Fig 1b) and the well density (number of wells per squared kilometer) was computed using a 25 km^2 grid over the Eagle Ford play on a yearly basis. The grid cell size was defined to improve the visual representation, since spatial results at finer scales were unreadable. Furthermore, subsurface area required by a single well was computed considering the horizontal length and the lateral separation in relation to adjacent boreholes:

$area = l * d$ (5)

where l is the horizontal length and d is the mean perpendicular distance between two consecutive horizontal segments in a well pad (see horizontal segments at Fig S1).

RESULTS AND DISCUSSION

FracFocus Data Analysis

FracFocus Data Mining.

During the analyzed period (2011-2017), 17,568 new wells were registered across the Eagle Ford play; nevertheless, only 15,033 wells (~85%) reported HF water use. The missing values corresponds to the period 2011-2012, as operators used an older format that was incompatible with the current database (Scanlon et al., 2017). During this period, annual drilled wells in FracFocus dataset increased from 69 in 2011 to 4,312 in 2014 (the drilling peak year) and decreased to 1,742 in 2017.

FracFocus showed a mean water use (TBW) of 25,134 m^3/well and a standard deviation of ~15,970 m^3, with an interquartile range (25^{th}-75^{th}, IQR) of ~14,660 and ~32,300 m^3 and a median of ~22,690 m^3. This dataset reported maximum values of TBW, well vertical depth (TBV), and days required for hydraulic fracturing (FracJob) of ~376,200 m^3/well, ~887,300 m and 935 days, respectively. By using the initial filter to detect evident outliers, 2,328 wells were removed from the original dataset. As a result, the TBW 25^{th}, 50^{th} and 75^{th} percentiles and mean value increased by ~2,000 m^3 while standard deviation remained unchanged (<5%). Maximum TBW decreased to ~127,500 m^3/well and maximum TVD decreased to 6,100 m.

Fig 2 shows the difference of univariate outlier detection (red dots) and the distribution of true data as violin plots, where the dashed lines represent the lower and upper quartiles. Percentile-based methods detected the higher number of outliers and reduced the long tails on the statistical distributions of TBW, TVD, and FracJob. The MAD method removed ~50% of wells due to the skewed distribution of TBnW values. On the other hand, 3STD is a less restrictive method for outlier recognition, even though long tails of TBnW, TVD, and FracJob remained on the distributions. Overall, the 2STD method showed similar behavior of TBnW and TVD when compared to the PCTL90 method.

[Insert Fig 2 here]

The multivariate outlier detection summary is shown in the Online Resource (Table S2). A total of 1,705, 3,255, 2,936, 260 and 953 wells classified as outliers were detected using the PCTL95, PCTL90, MAD, 3STD and 2STD methods, respectively. We selected the PCTL95 method as the more suitable option for the FracFocus dataset, when compared to other techniques. because it removed the minimum number of records to avoid the tailed distributions.

Statistics on the FracFocus database after the multivariate outlier detection using PCTL95 are shown in Fig 3. The Anderson-Darling test (Anderson and Darling, 1954) suggest that the statistical distributions of the analyzed variables follow a non-normal distribution (A^2=227, 3,996, 92, and 318 for TBW, TBnW, TVD, and FracJob, respectively). TBW showed a positively skewed bimodal distribution that ranged from ~5,500 to ~65,900 m^3/well, with a median value of ~24,400m^3/well and an IQR of 16,900 m^3. TVD shows a bimodal distribution that ranges from ~1,900 to ~4,200 m. Finally, FracJob indicates that the time of fracturing can last from 1 to 27 days after the perforation, with the higher number of wells fractured in the range of 4 to 10 days. Full statistics can be consulted in Table 2.

[Insert Fig 3 here]

To avoid reducing water volumes determined during the HF water footprint analysis, wells detected as outliers were replaced by the median value of the sample set, as no correlation was found between TBW and other variables (ρ<0.3). Records removed because of missing values were not considered in the procedure. Therefore, only the 1,706 wells identified as outliers were filled (~13% of final number of wells), having a poor impact on statistics, hence we use these records to increase the sample size. Filled dataset statistics are shown in Table 2.

[Insert Table 2 here]

HF Water Footprint using FracFocus.

HF water footprint analysis was conducted by (1) production zones and (2) analyzing the temporal evolution. Table 3 summarizes the statistics using the FracFocus database by production window; note that dry gas zone was omitted because only 208 wells were found (1.63% of the total wells), and thus contribution to total water volume during the period 2011-2017 was less than 2%. Mean TBW for oil and wet gas zones was calculated as 27,700 m^3/well and 24,700 m^3/well, respectively. Despite that median TBW (~24,300 m^3/well) is similar in magnitude in both oil and wet gas zones, results suggest that the TBW oil and wet gas distributions are statistically different, according to the alternative hypothesis by means of the Mann-Whitney test ($F=526072$, $p<0.05$). This is in accordance with previous studies in the Eagle Ford play (Hernández-Espriú et al., 2019). The TBW used for oil and wet gas windows showed a positive skew distribution (0.87 and 0.84, respectively) and kurtosis values of 3.44 and 4.6 (see Fig S2a).

[Insert Table 3 here]

HF water use in Eagle Ford play have been increasing over time, with a rising rate of ~1,900 m^3/well/year (Fig 4). The Kruskal-Wallis test revealed that medians from 2011 to 2017 varied statistically according to the rejected null hypothesis ($K=1644$, $p<0.001$). In 2011, median TBW was ~15,000 m^3/well with an IQR of 12,400-18,740 m^3/well; by 2017, median TBW increased to ~26,800 m^3/well and the IQR increased to 24,350-41,600 m^3/well. In 2017, for instance, ~36% of the wells exhibited a water use around the 75th percentile, that is, ~38,000 m^3. The results show that TBW has been increasing in similar proportion for both production zones (see Fig S2), but the 25th and 75th quartiles within the oil zone are ~20% higher than the wet gas window.

[Insert Fig 4 here]

During the analyzed period, total water volume to satisfy HF stimulation, before and after the data cleaning process, was computed as ~378 and ~331 Mm^3, respectively. Overall, oil and wet gas zones contributed in similar proportion to the total HF water volume (~48 and ~50.5 Mm^3, respectively). Historical evolution of accumulated HF water use and total number of stimulated wells per year across the Eagle Ford play are shown in Fig 5, where the effect of replacing outliers with median values was compared against the original dataset. Peak HF water use was observed in 2014, where original (red), filtered (green) and filled (blue) databases exhibited a volume of ~100 Mm^3. A similar number of wells was observed on original and filled databases for 2014 (~4,150 wells), except for the database without outliers, which contained ~13% fewer records than the original dataset.

Removed outliers during the first two years reduced the water volume from 13.12 Mm^3 to ~3 Mm^3 (original and filled datasets), with 863 and 181 wells drilled, respectively. Outliers statistics by method are showed on Online Resource, Table S2. Meanwhile, during 2017, HF water volume was 20% less after the filling-data procedure, with respect to the original dataset (~73 Mm^3) despite that in both cases, the total number of wells are similar (~1,740).

[Insert Fig 5 here]

IHS Data Analysis

IHS Data Mining

Data quality issues were observed when comparing TBW between IHS and FracFocus datasets (Fig S3). Well records in both datasets for TBW > 1,000 m^3 exhibited good correlation (ρ=0.88); nevertheless, ~13,400 IHS records reported a value of zero (see original IHS statistics in Table S3). FracFocus, on the other hand, reported water volumes from 500 to 68,000 m^3. Similar inconsistencies were highlighted by Scanlon et al. (2017) in the Permian Basin, attributed to operator errors related to unit inconsistencies.

To fix TBW in IHS, correlation and regression analyses were carried out using well records with TWB ≥ 1,000 m^3. We found that proppant, horizontal length, and FracFocus TBW were good predictors for assessing IHS TBW (r^2=0.61, 0.31 and 0.97, and regression slopes of 0.005, 16.395 and 0.994, respectively; Fig 6). Despite the good performance of FracFocus as predictor, the proppant regression model was used to fill TBW because several wells in IHS were not contained in FracFocus registry (~8,700 wells, ~47% of total IHS records). Thus, a total of 17,230 wells were filled with the proppant regression model (~92% of the wells contained in original dataset) and TBW 25th and 75th percentiles changed to 24,760 and 35,000 m^3/well, with a median of ~29,200 m^3 (Table S3).

[Insert Fig 6 here]

Multivariate outlier detection for IHS database suggest that the MAD method identified the smallest number of wells as outliers (1,554) when compared to PCTL90 and 2STD (~1,900 and ~3,300 outliers, respectively). In addition, the MAD method allowed us to remove the long tails on the statistical distributions when compared to the PCTL95 and 3STD techniques (Table S4).

[Insert Table 4 here]

Statistical distributions of the IHS dataset after removing outliers using the MAD method (Fig 7), show that TBW ranged from ~7,950 to ~51,500 m^3/well with a median of ~28,900 m^3/well (~18% higher than FracFocus). Proppant showed a positive skew distribution, with values of ~1,770, ~2,600 and ~3,790 ton/well (25th, 50th, and 75th percentiles, respectively). IQR values for horizontal length were estimated as ~1,770 and ~2,260 m with a median of ~1,990 m. The ratios of water use/length of lateral, proppant use/water use, and proppant use/length of lateral displayed medians of ~14.7 m^3/m, ~92.9 kg/m^3 and ~1,384 kg/m, respectively (Table 4). Statistics for the filled dataset remained similar to the dataset without outliers; nevertheless, the ~1,500 filled values represented an increase of ~44.6 Mm^3 compared to the HF water volume for the period 2011-2017 (~10% more water than the dataset without outliers).

[Insert Fig 7 here]

HF Water Footprint using IHS Dataset

Following the unconventional well classification described in the Online Resource (Table S1), we found that only ~590 wells were cataloged within the unconventional vertical class (~3.5% of the total wells). Statistics of unconventional horizontal and vertical wells (Table 5) show that the number of horizontal wells increased from 2,012 in 2011, to 4,038 in 2014, and then decreased to 910 wells in 2016. The number of unconventional vertical wells was almost constant from 2011 to 2014; however, well drilling decreased from ~140 in 2014 to 24 in 2016.

Results suggest that unconventional horizontal wells in the Eagle Ford play used, on average, ~42% more water for hydraulic fracturing when compared to unconventional vertical wells (~30,000 and ~21,150 m^3/well, respectively). Similar to FracFocus, a positive trend on TBW was observed in the IHS dataset, where water use in unconventional horizontal wells showed an increase of ~2,000 m^3/well/year and unconventional vertical wells showed an increase of ~440 m^3/well/year.

Furthermore, unconventional vertical wells were found to require ~30-50% of the proppant per cubic meter of water during the hydraulic fracturing, when compared to horizontal wells (~31 and 94 kg/m^3, respectively).

[Insert Table 5 here]

Results showed that the median proppant use has been increasing from ~1,940 ton/well in 2011 to ~3,700 ton/well in 2016, with an increasing trend of ~360 ton/well/year. Violin plots (Fig 8) revealed that during the last years, a higher amount of proppant use was observed for more wells. For instance, the difference of 75th and 50th quartiles were ~690 ton/well in 2011 and increased to ~1,350 ton/well in 2016.

The median horizontal lateral length remained almost constant over time, with a value of 1,980 m. The Kruskal-Wallis test suggested that distribution over time differs statistically ($K=627$, $p<0.001$). Median value of proppant use/water use increased from 83 kg/m^3 in 2011 to 110 kg/m^3 in 2016 and it was observed that the shape of the statistical distribution changed from a centered (mean ≈ median) to bimodal, respectively (Fig 8). Moreover, median HF water volume per horizontal length remained relative constant over time (~14.6 m^3/m); nevertheless, the mean increased from ~12.8 m^3/m in 2011 to ~16.2 m^3/m in 2016. This behavior could indicate that operators have been experimenting at a field level to increase production by injecting more water.

[Insert Fig 8 here]

Total HF water use associated with 17,230 unconventional wells for the period 2011 to the first half of 2017, considering the database filled by the regression model, was ~525 Mm^3. Outlier removal led to a reduction of ~ 68 Mm^3 (~13%) and the filled database reported a reduction of ~4% of water use, compared to the original database.

In accordance with the FracFocus database, a larger number of outlier wells were detected during the last years (~1,000 wells during the period 2014-2016). HF water use peaked in 2014 with an estimated volume of ~130 Mm^3 associated with ~4,180 wells (Fig S4). Furthermore, total HF water volume during the period 2011-2013 was ~10% higher than water volume during 2014-2016 (~254 and ~231 Mm^3, respectively). Yet, the number of wells decreased by ~30% during 2014-2016 compared to 2011-2013 (7,220 and 9,430 wells, respectively).

IHS vs FracFocus

HF Water Footprint

The Mann-Whitney test suggested that TBW was statistically different between datasets ($U=77x10^6$, $p<0.001$), where 25th, 50th and 75th percentiles of TBW in FracFocus were ~30, ~15 and ~5% lower than TBW from IHS (Tables 2 and 4). Considering wells with the same API number, median TBW in FracFocus was ~19% lower than IHS dataset (~24,300 vs ~29,900 m^3/well, respectively). The larger differences were observed during 2012-2013, when the median value of TBW in records from the FracFocus dataset were ~45% lower than IHS and ~19% lower during 2014-2016. We suggest that such differences were mainly associated with the filling step using linear regression with proppant as predictor, considering that correlation coefficient decreased from 0.88 (considering TBW>1,000 m^3/well) to ~0.5.

Accumulated HF water use from FracFocus during 2011-2017 was ~13% and ~28% lower than IHS database (~331 and ~503 Mm^3, respectively) (Table S5). Note that wells in the FracFocus dataset included those in the play "tail" (as seen in Fig 1), and that these wells were not available in IHS dataset. However, HF water use in this portion of the play is unimportant, because it represents only ~6% of the water volume reported in the FracFocus dataset during the production period 2011-2017.

The largest discrepancy between both data sources was observed during 2011-2013, during which time FracFocus and IHS reported ~3,000 vs ~9,000 wells, and a total HF water volume of ~60.5 and ~254 Mm^3, respectively. Similar results were detected within the 2014-2016 period. Water volume used for hydraulic stimulation during 2011-2017 was equivalent to ~57% and ~86% of the total groundwater (GW) withdrawals in 2016, play-wide, considering FracFocus and IHS datasets, respectively. In 2016, total HF water from FracFocus and IHS represented ~7.4% and ~5.4% of total withdrawal. By way of comparison, GW abstractions to satisfy irrigation and municipal demands totaled ~13.6% and ~9.8%, or ~24.6% and ~17.8% of total GW withdrawals, respectively.

HF Spatial Development

Maximum well density for the study period was estimated in 3.7 and 3.4 wells/km^2 considering FracFocus and IHS datasets, respectively. Well distribution tends to follow the geological limit between the oil and wet gas windows (see Figs 9a and b). For instance, higher number of wells (2,835, 2,697, 2,695 and 1,667 wells from IHS) in Karnes, Dimmit, La Salle and McMullen counties, respectively (Table S6). Overall, 25th, 50th and 75th percentiles ranged between 0.04, 0.12 and 0.24 wells/km^2, whereas, IHS IQR values were 0.08, 0.16 and 0.28 wells/km^2, at a yearly basis (Fig 9c). On the other hand, maximum well density determined from the FracFocus dataset was 1.68 wells/km^2/yr (2014), while maximum density from IHS was observed in 2015 (1.88 wells/km^2/yr).

According to Eq. 5, ground area required for a well depends of their pipeline lateral length and the separation between pipelines. From the 3D borehole reconstruction using the IHS down-hole survey data, we estimate that median lateral length (l) for the analysis period was computed as ~1,990 m and mean pipelines perpendicular distance (d) was estimated as ~170 m (detailed information about the d estimation is showed in Online Resource, Fig S1). Whereas, Ikonnikova et al. (2017) showed a value of perpendicular separation (d) of 180 m. Therefore, subsurface area for a single well is ~0.34 km^2. At play scale, total area required for FracFocus wells from 2011 to 2017 was ~4,300 km^2, that represented ~9.2% of total play area, while IHS wells covers an area of ~5,800 km^2 (~12.5% of total play area).

[Insert Fig 9 here]

Discussion

TBW estimated in this study is consistent with previous works in the Eagle Ford Formation. Nicot and Scanlon (2012) reported a median TBW value of 16,100 m^3/well from 1,040 wells during 2009-2011 period using the IHS dataset, compared to our 2011 median value of ~15,000 and ~24,200 m^3/well, derived from FracFocus and IHS using 48 and 2,012 wells, respectively. Gallegos et al. (2015) reported between 10,000-36,620 m^3/well for 2011-2014 and Chen and Carter (2016) showed a range of 8,000-120,000 m^3/well for 2009-2014, compared to our min-max range of 5,500-65,900 m^3/well for the study period (2011-2017). In addition, Kondash and Vengosh (2015) reported 13,700 and 15,060 m^3/well for wet gas and oil production zones during 2012-2014, whereas, Hernández-Espriú et al. (2019) 30,000 and 25,500 m^3/well for 2015-2017, respectively. In addition, Kondash et al. (2018) reported ~20,360 and ~31,070 m^3/well in 2015. Likewise, our results for the oil and wet gas production zones in 2015 indicate 24,350 and 28,030 m^3/well, respectively.

The lateral length and the amount of proppant used to stimulate unconventional wells are highly correlated with TWB (Fig 6). Furthermore, proppant use was observed as the best predictor of increased water use during the last years across the play, because proppant load and TBW followed similar temporal patterns (Figs. 4 and 8). Increasing of both proppant amount and lateral length coincided to the oil price drop at the beginning of 2015 (from ~80 to ~60 $/barrel), when producers moved to higher productivity areas. To increase energy production per well, operators injected more proppant and water, drilled longer laterals on horizontal boreholes and developed more fracturing stages to reduce the number of new wells (Ikonnikova et al., 2017). Within the latter, TBW increased by ~35% in 2017 compared to water volumes in 2014.

The higher number of outliers was observed at the initial and final years (2011-2012, 2017, respectively), associated with the lack of data quality during the first years on FracFocus and due to the increasing water demand for hydraulic fracturing within the last years.

Outliers in both FracFocus and IHS datasets represented ~23% and ~13% of the total HF water volume during 2011-2017, respectively. Accuracy of HF water volume estimates is crucial, particularly when compared with other water users. We found that HF water use during the peak year (2014) was ~17-22% of the total groundwater abstractions, play-wide. Scanlon et al. (2014) reported an estimate of 13% for 2013.

We estimate that a producing well in the Eagle Ford requires an average subsurface area of 0.34 km^2. Play-wide, current subsurface area covered by HF activities remains low (<10%) but is expected to increase over time. HF development projections proposed by Scanlon et al. (2014) and Ikonnikova et al. (2017) showed that between ~62,000 to ~87,000 new wells are anticipated over the next 20 years.

SUMMARY AND CONCLUSIONS

A multivariate outlier detection approach was tested to improve the assessment of water use for hydraulic fracturing (HF) in the Eagle Ford play, Texas. We used the following techniques: interquartile range at 95% (PCTL95), interquartile range at 90% (PCTL90), the median absolute deviation (MAD), Z-score with three times the standard deviation (3STD) and Z-score with two times the standard deviation (2STD). These approaches were tested using the FracFocus and IHS databases to compare the effect of data quality on the space-time HF development. Following our main objectives, we concluded that:

1) The PCTL95 and MAD are the two most feasible methodologies to clean the FracFocus and IHS databases, because they removed the long-tailed statistical distributions while preserving a higher number of records as outlier-free data, when compared to the other three techniques (PCTL90,

3STD and 2STD). Data cleaning is a vital process, particularly when estimating the mean, standard deviation, minimum and maximum values; thus, outlier detection is required to improve the space-time correlation between variables, patterns, and trends. At the same time, outliers represented an important water volume that must be considered when comparing with other water demands (municipal, irrigation, industrial).

2) FracFocus and IHS showed good correlation in TBW (~0.8); nevertheless, IHS presented irregular records associated with values lower than 1,000 m^3. HF water use from FracFocus was consistent with previous works, whereas IHS reported ~19% more water per well. Moreover, IHS provided additional information to improve the understanding of the HF water footprint.

3) HF water use per well was found highly correlated with the proppant load and horizontal length, where temporal variation in proppant use may explain the increase in HF water requirements. For practical purposes, horizontal lateral length combined with water use intensity per length has been used to generate scenarios, but proppant amount could be a better predictor of HF water use requirements.

4) Space-time evolution of HF development in the Eagle Ford play was described in terms of well density, subsurface area required for production, and HF water use and related variables (lateral length, proppant amount, vertical depth). We note that development also varies by production zone and well technology. Intensification of drilling and stimulation unconventional wells across the play indicated that wells concentrated over small regions would have a larger impact on local water resources, compared to a higher number of wells distributed over a larger region.

5) The framework presented here can be applied in other shale plays to improve estimates of HF water use footprint and to extract key factors to project future HF scenarios in emergent and early-stage plays, worldwide, with similar conditions.

ELECTRONIC SUPPLEMENTARY MATERIAL

Additional supporting information may be found online under the Supporting Information tab for this article: extra methodology description, additional results of outlier detection and complete statistics computed, among others.

CONFLICT OF INTEREST

The authors declare that they have no conflict of interest.

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REFERENCES

Anderson TW, Darling DA (1954). A Test of Goodness of Fit. Journal of the American Statistical Association. doi:10.1080/01621459.1954.10501232.

Arciniega-Esparza S, Breña-Naranjo JA, Hernández-Espriú A, Pedrozo-Acuña A, Scanlon BR, Nicot, Young MH, Wolaver BD, Alcocer-Yamanaka VH (2017). Baseflow Recession Analysis in a Large Shale Play: Climate Variability and Anthropogenic Alterations Mask Effects of Hydraulic Fracturing. Journal of Hydrology 553. doi:10.1016/j.jhydrol.2017.07.059.

Atkinson GM, Eaton DW, Ghofrani H, Walker D, Cheadle B, Schultz R, Shcherbakov R, Tiampo K, Gu J, Harrington RM, Liu Y, van der Baan M, Kao H (2016). Hydraulic Fracturing and Seismicity in the Western Canada Sedimentary Basin. Seismological Research Letters 87:631–647.

Barbato G, Barini EM, Genta G, Levi R (2011). Features and Performance of Some Outlier Detection Methods. Journal of Applied Statistics 38:2133–2149.

Barth-Naftilan E, Aloysius N, Saiers JE (2015). Spatial and Temporal Trends in Freshwater Appropriation for Natural Gas Development in Pennsylvania's Marcellus Shale Play. Geophysical Research Letters 42:6348–6356.

Chen H, Carter KE (2016). Water Usage for Natural Gas Production through Hydraulic Fracturing in the United States from 2008 to 2014. Journal of Environmental Management 170:152–159.

Conrad O, Bechtel B, Bock M, Dietrich H, Fischer E, Gerlitz L, Wehberg J, Wichmann V, Böhner J (2015). System for Automated Geoscientific Analyses (SAGA) v. 2.1.4. Geoscientific Model Development. doi:10.5194/gmd-8-1991-2015.

ESRI (2013). ArcGIS Desktop: Release 10.2. Redlands CA.

Frohlich C (2012). Two-Year Survey Comparing Earthquake Activity and Injection-Well Locations in the Barnett Shale, Texas. Proceedings of the National Academy of Sciences 109:13934–13938.

Galdeano C, Cook MA, Webber ME (2017). Multilayer Geospatial Analysis of Water Availability for Shale Resources Development in Mexico. Environ. Res. Lett.:12.

Gallegos TJ, Varela BA (2015). Trends in Hydraulic Fracturing Distributions and Treatment Fluids, Additives, Proppants, and Water Volumes Applied to Wells Drilled in the United States from 1947 through 2010 Data Analysis and Comparison to the Literature. doi:10.3133/ds868.

Gallegos TJ, Varela BA, Haines SS, Engle MA (2015). Hydraulic Fracturing Water Use Variability in the United States and Potential Environmental Implications. Water Resources Research 51:5839–5845.

Goodwin S, Carlson K, Bai B, Rein L, Knox K, Douglas C (2013). Improved Water Use Estimates for Drilling and Hydrualic Fracturing in Northeastern Colorado. Journal of Water Resources and Protection 2013:1262–1267.

Green RT, Winterle JR, Prikryl JD (2008). Discharge from the Edwards Aquifer through the Leona River Floodplain, Uvalde, Texas. Journal of the American Water Resources Association 44:887–901.

Guo M, Lu X, Nielsen CP, McElroy MB, Shi W, Chen Y, Xu Y (2016). Prospects for Shale Gas Production in China: Implications for Water Demand. Renewable and Sustainable Energy Reviews 66:742–750.

Hernández-Espriú A, Wolaver B, Arciniega-Esparza S, Scanlon B, Young MH, Nicot JP, Macías-Medrano S, Breña-Naranjo JA (2019). A Screening Approach to Improve Water Management Practices in Undeveloped Shale Plays, with Application to the Transboundary Eagle Ford Formation in Northeast Mexico. Journal of Environmental Management.

Homer CG, Dewitz JA, Yang L, Jin S, Danielson P, Xian G, Coulston J, Herold ND, Wickham JD, Megown K (2015). Completion of the 2011 National Land Cover Database for the Conterminous United States-Representing a Decade of Land Cover Change Information. Photogrammetric Engineering and Remote Sensing 81:345–354.

Horner RM, Harto CB, Jackson RB, Lowry ER, Brandt AR, Yeskoo TW, Murphy DJ, Clark CE (2016). Water Use and Management in the Bakken Shale Oil Play in North Dakota. Environmental Science and Technology 50:3275–3282.

Howell DC (1998). Statistical Methods in Human Science. New York: Wadsworth.

Huber PJ (1981). Robust Statistics. doi:10.1002/9780470434697.

IHS Energy (2011). Petroleum Information Data Model (PIDM) 2.5 Data Management System.

Ikonnikova SA, Male F, Scanlon BR, Reedy RC, McDaid G (2017). Projecting the Water Footprint Associated with Shale Resource Production: Eagle Ford Shale Case Study. Environmental Science and Technology 51:14453–14461.

Kondash AJ, Lauer NE, Vengosh A (2018). The Intensification of the Water Footprint of Hydraulic Fracturing. Science Advances 4. doi:10.1126/sciadv.aar5982.

Kondash A, Vengosh A (2015). Water Footprint of Hydraulic Fracturing. Environmental Science & Technology Letters 2:276–280.

Leys C, Ley C, Klein O, Bernard P, Licata L (2013). Detecting Outliers: Do Not Use Standard Deviation around the Mean, Use Absolute Deviation around the Median. Journal of Experimental Social Psychology 49:764–766.

Lin Z, Lin T, Lim SH, Hove MH, Schuh WM (2018). Impacts of Bakken Shale Oil Development on Regional Water Uses and Supply. JAWRA Journal of the American Water Resources Association 54:225–239.

McKinney W, Team PD (2015). Pandas - Powerful Python Data Analysis Toolkit. Pandas - Powerful Python Data Analysis Toolkit.

Miller J (1991). Reaction-Time Analysis with Outlier Exclusion---Bias Varies with Sample-Size. Quarterly Journal of Experimental Psychology, Section A---Human Experimental Psychology.

Nicot JP, Scanlon BR (2012). Water Use for Shale Gas Production in Texas, U.S. Environmental Science & Technology 46:3580–3586.

Oikonomou PD, Kallenberger JA, Waskom RM, Boone KK, Plombon EN, Ryan JN (2016). Water Acquisition and Use during Unconventional Oil and Gas Development and the Existing Data Challenges: Weld and Garfield Counties, CO. Journal of Environmental Management 181:36–47.

Oliphant TE (2007). SciPy: Open Source Scientific Tools for Python. Computing in Science and Engineering. doi:10.1109/MCSE.2007.58.

Pacsi AP, Sanders KT, Webber ME, Allen DT (2014). Spatial and Temporal Impacts on Water Consumption in Texas from Shale Gas Development and Use. ACS Sustainable Chemistry & Engineering 2:2028–2035.

Pedregosa F, Varoquaux G, Gramfort A, Michel V, Thirion B, Grisel O, Blondel M, Prettenhofer P, Weiss R, Dubourg V, Vanderplas J, Passos A, Cournapeau D, Brucher M, Perrot M, Duchesnay E (2011). Scikit-Learn: Machine Learning in Python. Journal of Machine Learning Research 12:2825–2830.

Pierre JP, Abolt CJ, Young MH (2015). Impacts from Above-Ground Activities in the Eagle Ford Shale Play on Landscapes and Hydrologic Flows, La Salle County, Texas. Environmental Management 55:1262–1275.

Python Software Foundation (2013). Python Language Reference, Version 2.7. Python Software Foundation. http://www.python.org.

QGIS Development Team (2015). QGIS Geographic Information System. Open Source Geospatial Foundation Project.

Rousseeuw PJ, Hubert M (2011). Robust Statistics for Outlier Detection. Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery. doi:10.1002/widm.2.

Scanlon BR, Duncan I, Reedy RC (2013). Drought and the Water–Energy Nexus in Texas. Environmental Research Letters 8:045033.

Scanlon BR, Reedy RC, Male F, Walsh M (2017). Water Issues Related to Transitioning from Conventional to Unconventional Oil Production in the Permian Basin. Environmental Science & Technology:acs.est.7b02185.

Scanlon BR, Reedy RC, Nicot JP 2014. Will Water Scarcity in Semiarid Regions Limit Hydraulic Fracturing of Shale Plays? Environmental Research Letters 9:124011.

Scanlon BR, Reedy RC, Nicot JP (2014). Will Water Scarcity in Semiarid Regions Limit Hydraulic Fracturing of Shale Plays? Environmental Research Letters 9:124011.

Schwartz MO (2015). Modelling the hypothetical methane-leakage in a shale-gas project and the impact on groundwater quality. Environmental Earth Sciences 73 (8): 4619–4632 DOI: 10.1007/s12665-014-3787-3

Seabold S, Perktold J (2010). Statsmodels: Econometric and Statistical Modeling with Python. Proc of the 9th Python in Science Conf.

Sharma S, Shrestha A, McLean CE, Martin SC (2015). Hydrologic Modeling to Evaluate the Impact of Hydraulic Fracturing on Stream Low Flows: Challenges and Opportunities for a Simulation Study. American Journal of Environmental Sciences 11:199–215.

Slonecker E, Milheim L, Roig-Silva C (2012). Landscape Consequences of Natural Gas Extraction in Bradford and Washington Counties, Pennsylvania, 2004–2010. US Geological Survey Open:2004–2010.

Thompson SJ, Johnson DH, Niemuth ND, Ribic CA (2015). Avoidance of Unconventional Oil Wells and Roads Exacerbates Habitat Loss for Grassland Birds in the North American Great Plains. Biological Conservation 192:82–90.

Trabucco A, Zomer RJ (2009). Global Aridity Index (Global-Aridity) and Global Potential Evapo-Transpiration (Global-PET) Geospatial Database. CGIAR Consortium for Spatial Information. http://www.csi.cgiar.org.

TWDB (2018). Historical Groundwater Pumpage Estimates. Historical Groundwater Pumpage. http://www.twdb.texas.gov/waterplanning/waterusesurvey/historical-pumpage.asp. Accessed 27 Sep 2018.

USEPA (2015). Assessment of the Potential Impacts of Hydraulic Fracturing for Oil and Gas on Drinking Water Resources. External Review:998.

Vengosh A, Jackson RB, Warner N, Darrah TH, Kondash A (2014). A Critical Review of the Risks to Water Resources from Shale Gas Development and Hydraulic Fracturing in the United States. Enviromental Science & Technology 16:15.

Vidic RD, Brantley SL, Vandenbossche JM, Yoxtheimer D, Abad JD (2013). Impact of Shale Gas Development on Regional Water Quality. Science 340:1235009.

Walker EL, Anderson AM, Read LK, Hogue TS (2017). Water Use for Hydraulic Fracturing of Oil and Gas in the South Platte River Basin, Colorado. JAWRA Journal of the American Water Resources Association 53:839–853.

Warner NR, Christie CA, Jackson RB, Vengosh A (2013). Impacts of Shale Gas Wastewater Disposal on Water Quality in Western Pennsylvania. Environmental Science and Technology 47:11849–11857.

Waskom M (2018). Seaborn: Statistical Data Visualization. Webpage.

Yu M, Weinthal E, Patiño-Echeverri D, Deshusses MA, Zou C, Ni Y, Vengosh A (2016). Water Availability for Shale Gas Development in Sichuan Basin, China. Environmental Science & Technology 50:2837–2845.

Williamson R, Esterhuyse S (2019). Expected wastewater volumes associated with unconventional oil and gas exploitation in South Africa and the management thereof. Bulletin of Engineering Geology and the Environment DOI: 10.1007/s10064-019-01579-y

Zhao Y (2012). R and Data Mining: Examples and Case Studies. Elsevier. http://www.rdatamining.com/books/rdm%5Cnhttp://linkinghub.elsevier.com/retrieve/pii/B9780123969637000015.

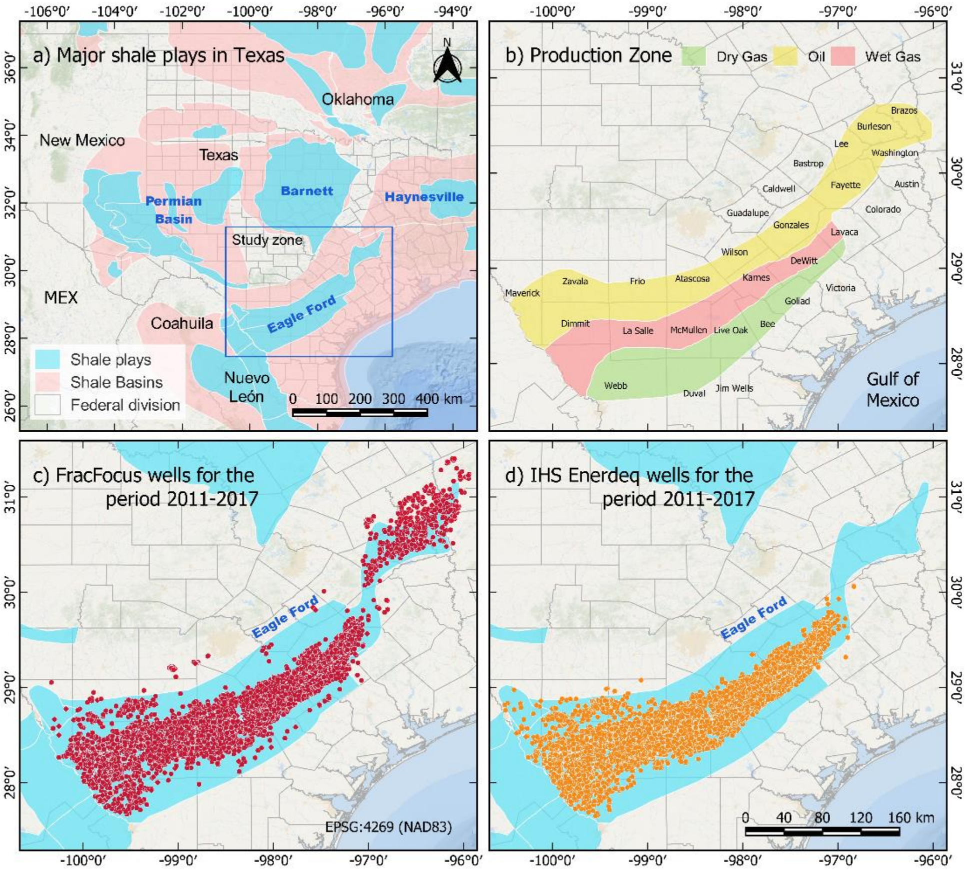

Fig 1 Study area location showing a) Major shale plays across Texas, b) The Eagle Ford play production zones, c) FracFocus wells across the Eagle Ford play (2011-2017), and d) IHS wells across the Eagle Ford play (2011- half-2017).

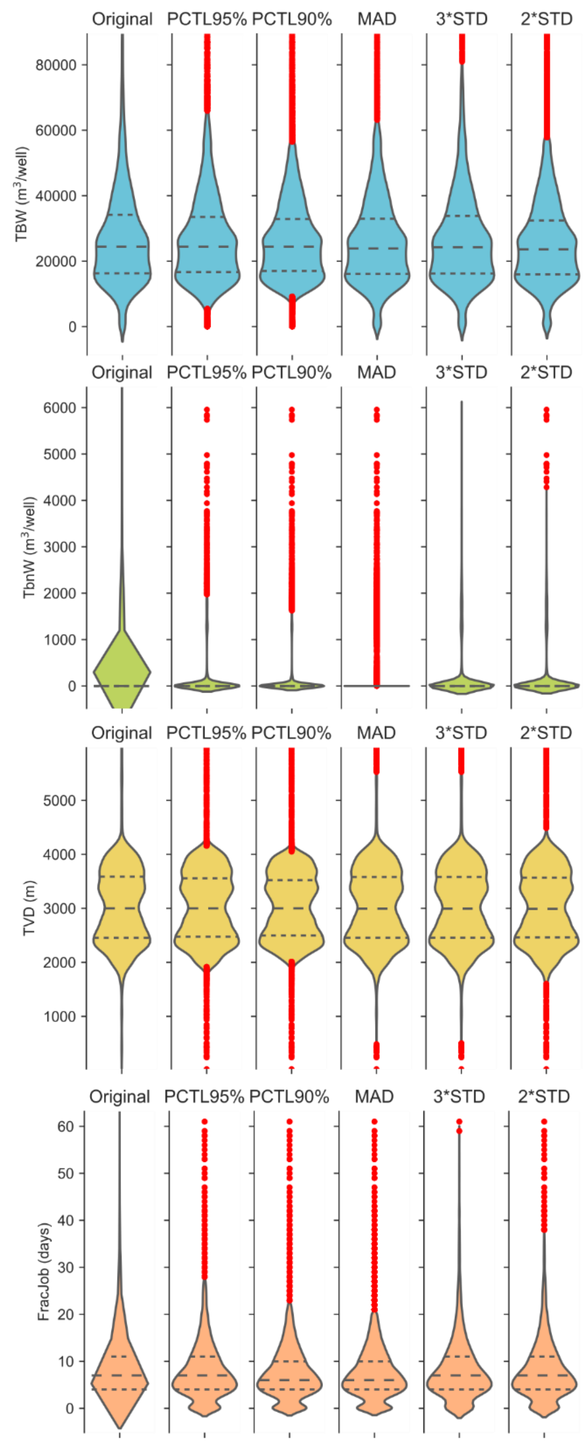

Fig 2 Univariate outliers' detection differences using FracFocus. Violin plots indicates the higher density values and dashed lines represent the interquartile range. Outliers are represented as red dots. Axis titles correspond to: Original, database with initial filter applied; PCTL95, interquartile range at 95%; PCTL90, interquartile range at 90%; MAD, median absolute deviation; 3STD, Z-score 3*std as threshold; 2STD, Z-score applied with 2*std as threshold. Variables on y-axis

correspond to: TBW, total base water volume for HF; TBnW, total base no water volume; TVD, true vertical depth of borehole; FracJob, number of days for hydraulic fracturing.

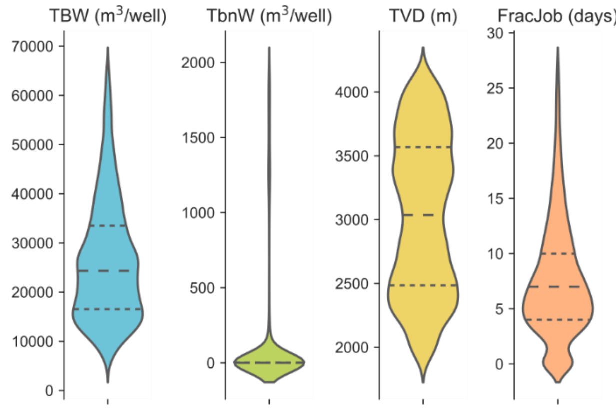

Fig 3 FracFocus statistics after removing outliers detected by interquartile range at 95% (PCTL95) method. TBW is the total base water volume for HF; TBnW, total base non water volume; TVD, true vertical depth of the borehole; FracJob, number of days for hydraulic fracturing.

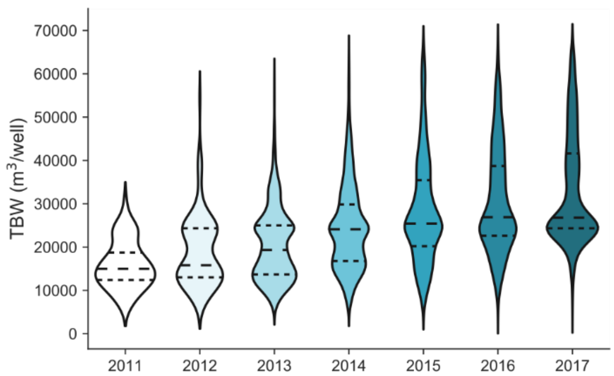

Fig 4 Annual evolution of FracFocus total base water volume for HF (TBW) for the period 2011-2017.

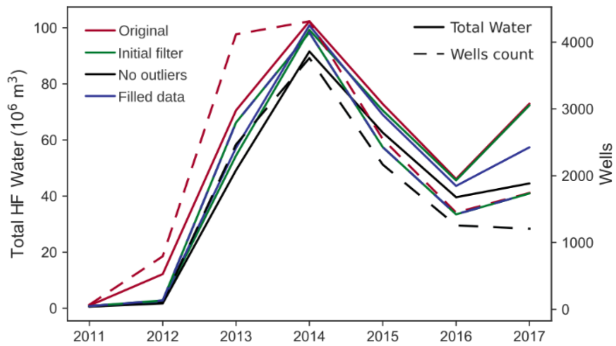

Fig 5 Annual evolution of total water required for hydraulic fracturing (left axis) and number of wells in FracFocus for the original dataset, initial filter, dataset without outliers and dataset filled with median values. Continuous lines correspond to HF water volume and dashed lines to wells drilled. Red line corresponds to database, green line to database after the application of the initial filter, black line to database without outliers and blue line to database where detected outliers were filled using the median HF water volume.

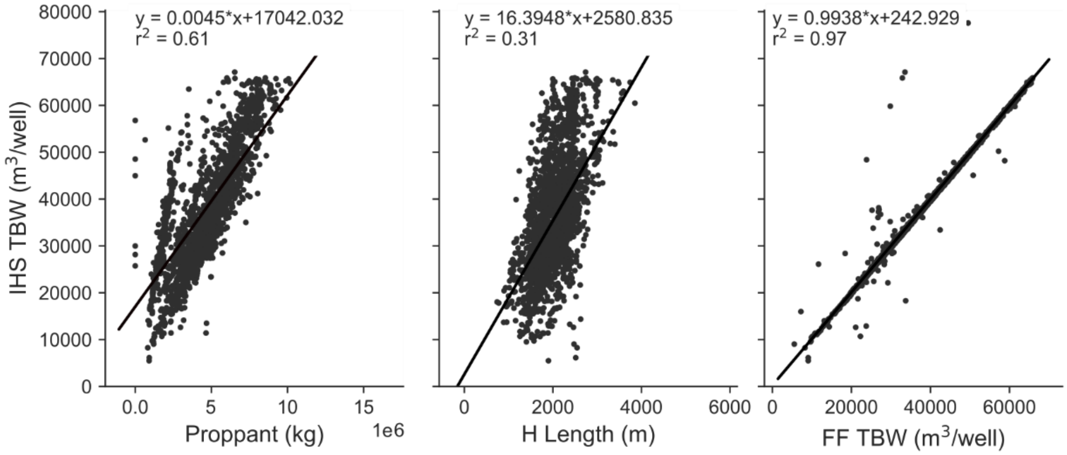

Fig 6 Correlation between IHS HF water volume (TBW) and proppant load (Proppant), well's horizontal length (H Length) and TBW from FracFocus for period from 2011 to half-2017.

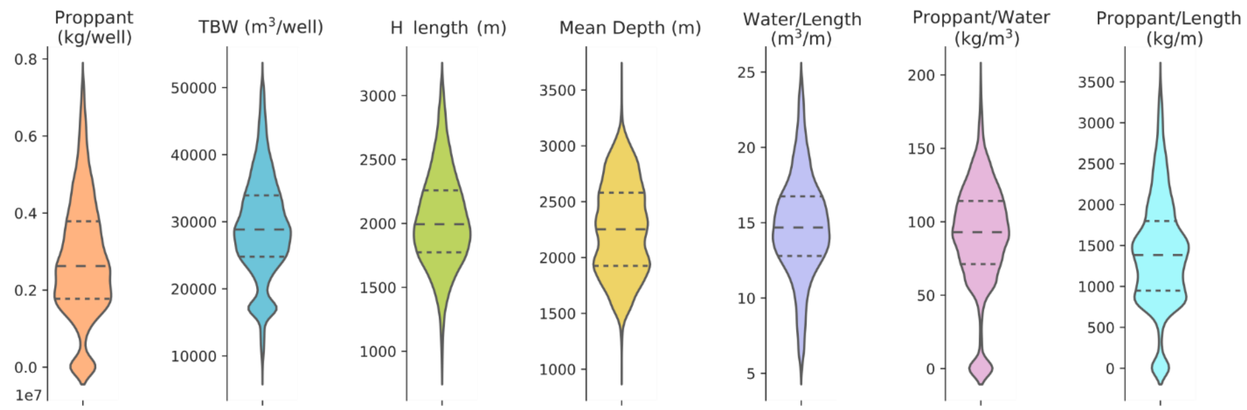

Fig 7 IHS statistics after removing outliers detected by the median absolute deviation (MAD) method for the period 2011 to half-2017. Proppant is the proppant load used during the fracturing stages; TBW is the total base water volume; H length is the horizontal length of the borehole; Mean Depth is the average depth of the horizontal segment of the borehole.

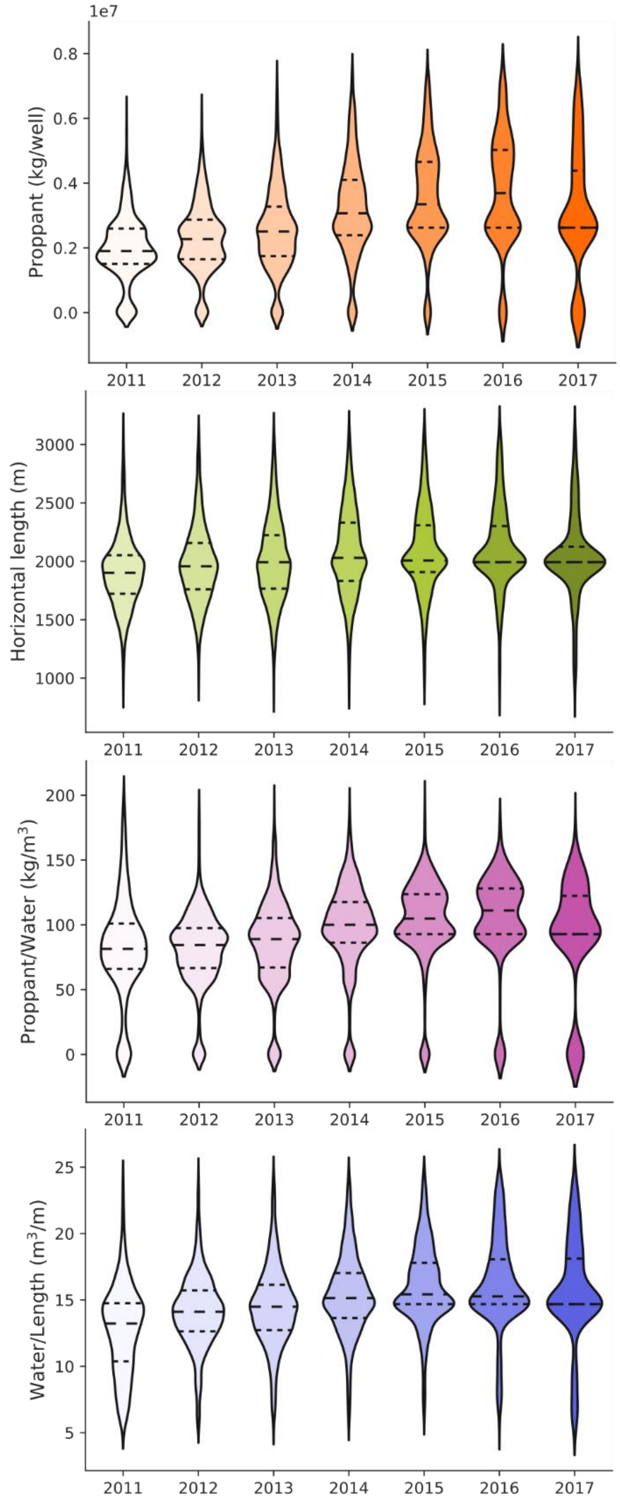

Fig 8 Annual evolution of IHS variables for the period 2011 to half-2017.

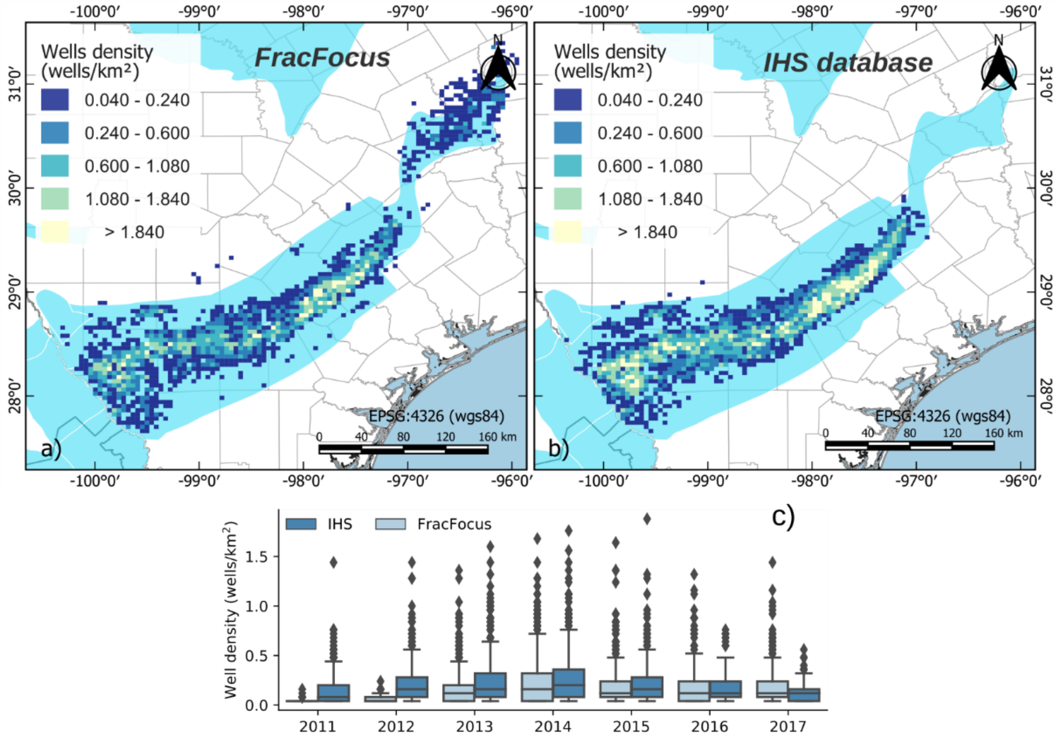

Fig 9 Well density for the period 2011-2017, considering a) FracFocus dataset b) IHS dataset, and c) temporal evolution of well density for both datasets across the play.

TABLES DESCRIPTION

Table 1 Description of the variables used in this study from FracFocus and IHS datasets

Database	Column name	Label[1]	Description
FracFocus	APINumber	API	10-digits well number identification provided by the American Petroleum Institute
	JobStartDate	Start	Initial date of HF activities
	JobEndDate	End	Final date of HF activities
	TVD	TVD	Well depth
	TotalBaseWaterVolume	TBW	Water volume used in the HF fluid
	TotalBaseNonWaterVolume	TBnW	Volume of no water components of the HF fluid
	FracDuration[2]	FracJob	Days required for the HF activities in a well, computed as End-Start+1
IHS	IWU	API	Same that API in FracFocus
	Date Spud	Start	Initial date of HF activities
	Date Completion	End	Final date of HF activities
	Hole Direction	Direction	Well orientation (vertical, horizontal)
	Final Status	Status	Show production status or dry well or abandoned
	Lat Len Horiz Displacement[3]	H Length	Horizontal well length
	Num Frac Stages	Stages	Number of fracturing stages
	Total proppant	Proppant	Weight of total proppant used
	Depth True Vertical[3]	TVD	Well depth
	Total Fluid	Fluid	Total volume of fluid used in the HF
	Total water volume[2]	TBW	Total water volume computed as the sum of Fluid/Water, Fluid - Slick Water and Fluid - Salt Water
	Total non-water volume[2]	TBnW	Difference between Total Fluid and Total water volume
	FracDuration[2]	FracJob	Days required for the HF activities in a well, coputed as End-Start+1

[1] Variable name used in this analysis

[2] Computed from variables contained in the databases

Table 2 FracFocus statistics (2011-2017) from the original dataset, after removing outliers with the interquartile range at 95% (PCTL95) method, and filling dataset using the median value. TBW is the total base water volume for HF; TVD is the true vertical depth of the borehole; TBnW is the total base non water volume; FracJob is the number of days for hydraulic fracturing

	Stats	TBW (m^3/well)	TVD (m)	TBnW (m^3/well)	FracJob (days)
Original stats	wells	15033	15035	13028	17568
	mean	25134	2953	240	7
	std	15973	7287	1994	13
	min	0	0	0	0
	25%	14663	2390	0	0
	50%	22681	2931	0	5
	75%	32335	3562	0	9
	max	376193	887327	88272	935
Statistics without outliers	wells	11001	11001	11001	11001
	mean	26344	3032	135	8
	std	12292	613	417	5
	min	5488	1916	0	
	25%	16549	2485	0	4
	50%	24345	3037	0	7
	75%	33490	3569	0	10
	max	65876	4156	1969	27
Statistics filled	wells	12706	12706	12706	12706
	mean	26075	3033	117	8
	std	11458	571	391	5
	min	5488	1916	0	0
	25%	17686	2543	0	4
	50%	24345	3037	0	7
	75%	31616	3481	0	10
	max	65876	4157	1968	27

Table 3 FracFocus statistics by production zone for the period 2011-2017. TBW is the total base water volume for HF; TVD is the true vertical depth of the borehole; TBnW is the total base non water volume; FracJob is the number of days for hydraulic fracturing

Zone	Stats	TBW (m^3/well)	TVD (m)	TBnW (m^3/well)	FracJob (days)
Oil	wells	5735	5735	5735	5735
	mean	27729	2905	141	7
	std	11906	537	430	5
	min	5488	1916	0	0
	25%	19549	2481	0	5
	50%	24345	2950	0	7
	75%	33987	3306	0	9
	max	65876	4145	1968	27
Wet Gas	wells	6763	6763	6763	6763
	mean	24720	3145	100	8
	std	10881	575	359	5
	min	5699	1930	0	0
	25%	16380	2591	0	4
	50%	24345	3119	0	7
	75%	29728	3634	0	10
	max	65848	4156	1962	27

Table 4 IHS statistics after removing outliers with the MAD method and for the filling dataset using the median value. Statistics correspond to the period 2011 to half-2017. TBW is the total base water volume; H length is the horizontal length of the borehole; Mean Depth is the average depth of the horizontal segment of the borehole

	Stats	**TBW (m^3/well)**	**Proppant (ton/well)**	**H Length (m)**	**TVD (m)**	**Water/Len (m^3/m)**	**Propp/Water (kg/m^3)**	**Propp/Len (kg/m)**
Statistics without outliers	wells	15676	15676	15085	15085	15085	15676	15085
	mean	29230	2803	2027	2260	14.76	89.96	1409
	std	7516	1536	371	413	3.38	36.98	673
	min	7941	0	850	985	5.26	0.00	0.00
	25%	24783	1774	1773	1926	12.79	71.17	948
	50%	28854	2625	1993	2253	14.68	92.87	1384
	75%	33932	3788	2259	2581	16.75	114.21	1800
	max	51499	7451	3147	3622	24.62	197.47	3534
Statistics filled	wells	17222	17222	16631	16631	16631	17222	16631
	mean	29196	2787	2024	2260	14.76	90.22	1407
	std	7172	1466	354	393	3.22	35.29	641
	min	7941	0	850	985	5.26	0.00	0
	25%	25213	1858	1797	1953	13.02	73.58	991
	50%	28854	2625	1993	2253	14.68	92.87	1384
	75%	33318	3628	2229	2548	16.53	111.87	1730
	max	51499	7451	3147	3622	24.62	197.47	3534

Table 5 IHS database mean values by year and by well class (unconventional horizontal and unconventional vertical) from 2011 to half-2017. TBW is the total base water volume; H length is the horizontal length of the borehole; Mean Depth is the average depth of the horizontal segment of the borehole

Well Class	Year	Number of wells	TBW (m^3/well)	Proppant (ton/well)	H Length (m)	Water/Len (m^3/m)	Propp/Water (kg/m^3)	Propp/Len (kg/m)
Horizontal	2011	2012	24196	2029	1906	12.82	84.13	1061
	2012	3329	27502	2343	1977	14.11	82.18	1181
	2013	3743	28544	2583	2005	14.48	86.23	1290
	2014	4038	31560	3277	2079	15.39	99.82	1583
	2015	2061	33154	3638	2093	16.05	105.79	1743
	2016	910	33860	3786	2119	16.22	106.11	1804
	2017	538	31432	3246	2042	15.69	95.07	1627
Vertical	2011	139	19717	889			41.78	
	2012	125	20352	800			33.51	
	2013	84	20959	868			31.07	
	2014	139	21825	1049			31.91	
	2015	52	18509	325			8.93	
	2016	24	25570	1891			52.33	
	2017	28	21145	872			21.47	