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Mining FracFocus and Production Data for Efficacy of Fracturing Fluid Formulations

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Abstract

Using environmentally friendly and low-cost chemical ingredients that are also effective in terms of oil and/or gas production is the ultimate goal of formulating fracturing fluids. The relatively transparent production data and fracturing fluid ingredients through FracFocus provide an opportunity to mine large amount of data for insights on the efficacy of fracturing fluid ingredients, which were not possible through traditional means of individual lab tests and statistical analysis of individual ingredients and small clusters of wells.

Here we showcase a big data analytics framework where through data preprocessing and feature engineering, algorithms and models can be built to quantify the efficacy factors of fracturing fluid ingredients for gas production. Special attention is paid to geological properties so that they are similar or identical for comparison.

As an example, we demonstrate the big data analytics process on a dataset of more than 3100 horizontal Marcellus shale gas wells in Pennsylvania, and the data-based insights not only corroborate the empirical wisdoms known in the industry, but also established quantitative measures such that ingredients with higher efficacy factors should be used more confidently, while caution should be exercised on those ingredients that have negative efficacy factors for gas production.

This work also shows the potential value of the FracFocus database in improving the efficiency and efficacy of hydraulic fracturing, in addition to its intended environmental cause. Big data and data sharing should be encouraged not only for public safety grounds, but also for economic reasons for the industry.

Introduction

A fracturing fluid type can make or break the production prospect of a well. For example, it has been reported that high viscosity slickwater was the most appropriate fracturing fluids to be used to achieve higher cumulative production over plain slickwater or cross linked fluids in 5 years for the Upper Wolfcamp in the Permian Basin. Fracturing fluid design is also a crucial factor in planning well trajectory placement (lateral landing). In other words, the fracturing design can significantly impact the well drilling quality, backwardly (SPE 190860).

Selecting competing ingredients for a fracturing fluid formulation is often based on cost reduction and HSE stewardship. As such, the industry has been exploring programs to assess chemicals based on risk factors supplemental to employee exposure and operational effectiveness. For example, Southwestern Energy installed a Right Products program for chemical selection and denied 18% of the 263 chemicals the company had been using (SPE 189891).

There has been numerous commercial studies on comparison of individual products that go into fracturing fluids, such as proppants, surfactants, friction reducers, and biocides. Often they are based on statistics of a small group of wells that used competitive products of the same or similar type or specification. A grain of salt should be used when interpreting the results as objectivity demands.

Objectively measuring the operational effectiveness of fracturing fluid ingredients have been difficult. An ingredient's efficacy to achieve its purported functionality may be compromised by its incompatibility with other ingredients [Jon Raymond, 2015]. It is prohibitively expensive, if not impossible, to evaluate fully formulated fracturing fluids in lab tests if they were to simulate the intricate and dynamic processes of temperature, pressure, shear history and chemical environments in the field. Instead, an ingredient's efficacy test often retreats to simplified basic types of fracturing fluids. An ingredient's efficacy can also be field dependent, as shown in [Saudi Aramco J. Of Tech. Winter 2015] that nitrate treatment cannot be replicated based on its performance in other fields.

As a result, formulations from the laboratory are often changed by the completion field engineers on the fly to meet engineering needs without sufficient laboratory validation. If the original fluid design is not robust enough for on-job-site changes, the effectiveness of each ingredient and the fracturing fluid as a whole can be significantly discounted.

Trends such as fracturing fluid type selection have been observed directly from FracFocus and by operators with large numbers of wells (SPE 163875), where the results resembles closely empirical knowledge about general trends of what has been happening in the field. Most notably is the notion to pump as much sand as possible to achieve higher productivity. But such studies lack the in-depth discovery of the connection between individual factors, i.e. fracturing fluid ingredients, and well productivity.

A promising approach to fracturing fluid optimization is big data analytics. This is increasing becoming possible and feasible as large volumes of data are becoming available, such as FracFocus which contains fracturing fluid formulations of about 130,000 fracturing operations. The regulatory nature of FracFocus program make it trust worthy, and combined with production data, the well can be viewed as the ultimate "lab" test for fracturing fluid efficacy.

Framework of Data Analytics

The framework of this work for efficacy of fracturing fluid ingredients is demonstrated in the following using a case study on 3126 selected wells horizontal Marcellus shale gas wells in the state of Pennsylvania. It is mostly a data pipeline and includes components of data collection, data cleaning and preprocessing, feature engineering and dataset preparation, modeling and visualization, in the order. Each of these pipeline components may have sub components that take in input data and generate output data to feed subsequent components. Each sub component shall be kept as small as possible for easy scale up and restructuring.

Also included in the framework is the understanding part that involves the user - physical interpretation of modeling results and validation to generate insights and leads, which in turn can be fed back into the data pipeline to continuously refine the data analytics framework.

Data Collection

FracFocus database [FracFocus] (SQL version in February 2018) and production data from Pennsylvania Department of Environmental Protection (PADEP) are raw data sources [PADEP] for modeling. Also the database of produced water chemistry (USGSPWDBv2.3) from the US Geological Survey (USGS) [USGS] is used as source data for interpretation and validation purposes.

Data Cleaning and Preprocessing

Though the best fracturing fluid formulation database the industry has ever seen, the FracFocus database is still under development for data cleaning and structuring before it can be properly used for analytics. It only "contains information exactly as reported to FracFocus, and only the data displayed on the disclosure PDF files". Subjective to human errors, data entries into disclosure PDF files could be mischaracterization or simply typos.

FracFocus data were transformed from SQL format into CSV files, which are then processed with Python programs to obtain the physical quantities of each ingredient for every fracturing fluid formulation using the following formula:

$$Quantity = 8.345 * TotalBaseWaterVolume * PercentHFJob / BaseWaterPercentHFJob$$

Total Base Water Volume is in gallons, the ingredient's percentage (% by mass) in hydraulic fracturing job is PercentHFJob, and base water's percentage is expressed by BaseWaterPercentHFJob. The physical quantity obtained has the unit of lbs.

Quoted from FracFocus, there are "Limitations of the Database":

1. "Because the % Mass of the additive will be expressed as its maximum concentration, the total % Mass of ingredient percentage may exceed 100%";
2. "The total may not equal 100% due to the absence of non MSDS ingredients which may or may not be listed depending upon state reporting requirements."

For the entries that have total % Mass of ingredient percentage exceeding 100%, and the total percentage not equal to 100%, they are excluded from the dataset of selected wells in the following procedure. Apparent typos and nonconformity in the source data were modified as appropriate. Raw data may be normalized and missing value may be treated as zero or ignored.

The minimum data period in PA production data is monthly. It is not uncommon that some wells only report biannual or annual production data. For this reason, average daily production data is used for modeling, instead of the more common initial production data.

Feature Engineering and Dataset Preparation

Much like the filters for database search engines, the dataset for modeling, a subset of the full database of fracturing fluid formulations and production data, was obtained by a set of qualifying conditions. For instance:

1. Wells in the dataset are horizontal wells producing gas from Marcellus shale in Pennsylvania;
2. Wells with total percentage of ingredients equal to 100% in the fracturing fluid formulation;
3. Wells with multiple fracturing operations, i.e. refract jobs on same wells with different JobEndDate values, are removed from the dataset;
4. Only gas production from PADEP's Production Report is included in the dataset for modeling.
5. Fracturing job end date of the wells in the dataset should be no later than June 30, 2017.

It is assumed that the reservoir and rock properties are the same or similar, such as reservoir permeability, distribution of natural fractures, pay thickness, Young's modulus, porosity, water saturation, bottom hole pressure, fracture toughness, fluid loss properties, reservoir temperature and pressure, drainage and interaction among neighboring wells, and the composition and properties of reservoir connate fluids. Also implied are that differences in treatment variables such as number of fracturing stages, injection rates, finer specifications of ingredients such as proppant mesh sizes, physical forms of biocides are insignificantly small. Although these may be big-if assumptions, we believe they provide a reasonable starting point for insights and refinement can be done within the pipeline with more and different types of filters than the ones listed in (1) – (5) above.

The final dataset contains quantities of ingredients of fracturing fluid formulations for 3126 wells, whose geographical distribution is shown in Figure 1.

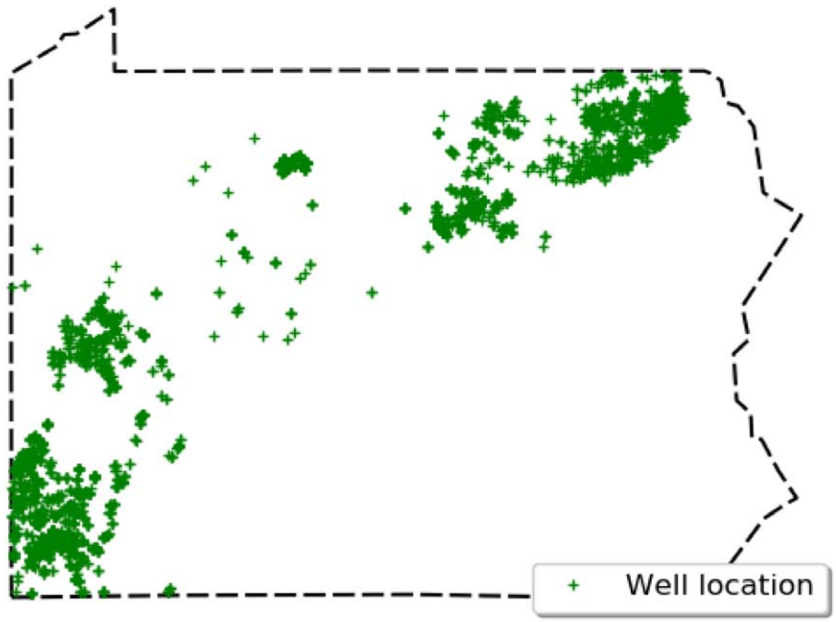


Figure 1—Locations of horizontal Marcellus shale gas wells used for modeling

Modeling and Visualization

Random forest/decision tree algorithms written in Python were used to learn models and patterns from the dataset prepared from Section 2.3 above. The immediate learned results are the efficacy factors between gas production from and the 324 ingredients used by the 3126 wells, as partly shown in Figures 2 and 3, and Tables 1 and 2.

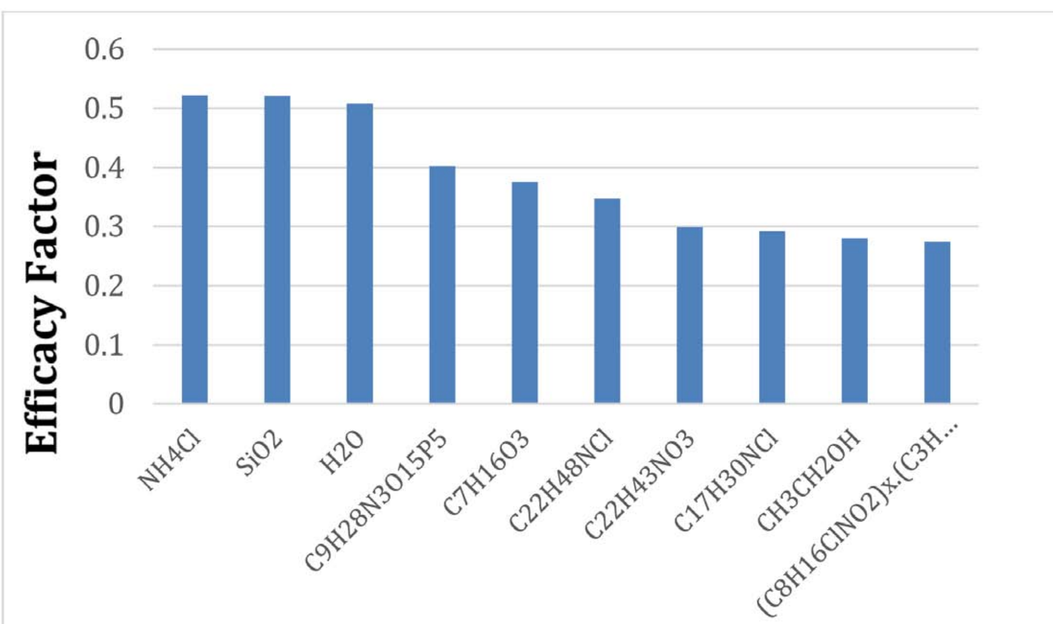


Figure 2—Ingredients with the highest positive efficacy factor for gas productivity

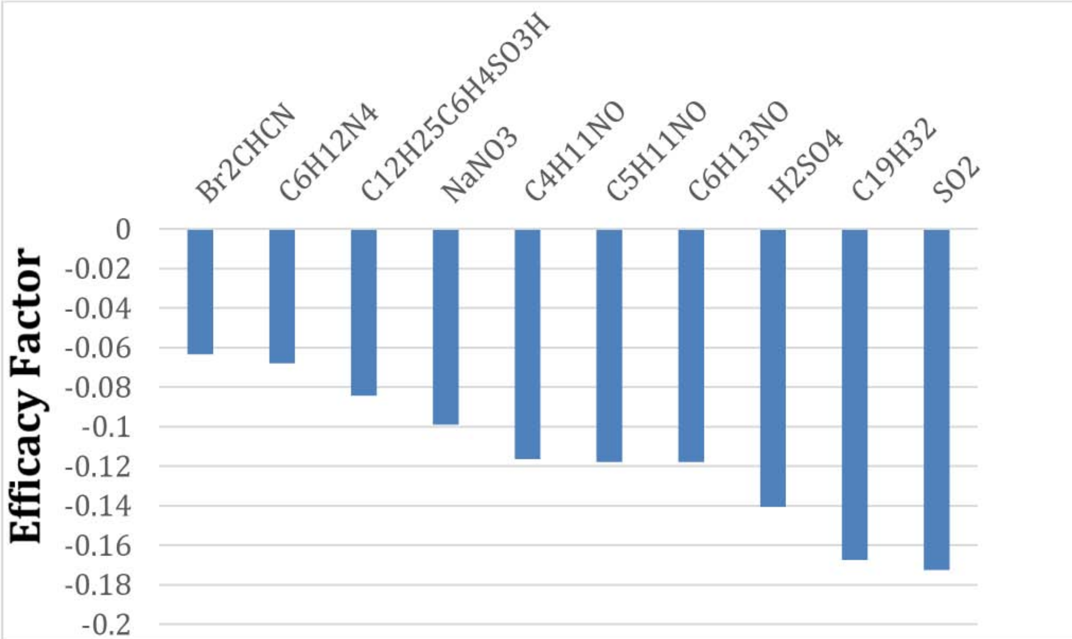


Figure 3—Ingredients with the most negative efficacy factor for gas productivity

Table 1—Ingredients with the highest positive efficacy factor with gas productivity

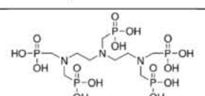
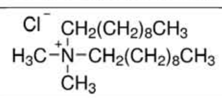
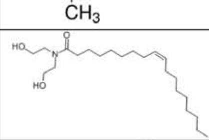
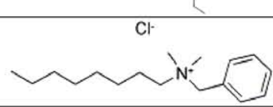
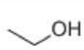
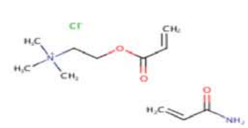
Chemical Name & CAS No.	Chemical structure	Chemical formula	Purpose	Efficacy factor	# wells using
Quartz (sand) CAS_14808-60-7	SiO2	SiO2	Proppant	0.531953	3126
Water CAS_7732-18-5	H2O	H2O	water	0.50126	3126
Ammonium Chloride CAS_12125-02-9	NH_4Cl	NH4Cl	friction reducer/scale inhibitor	0.490018	1214
Diethylenetriaminepentakis (methylphosphonic acid) CAS_15827-60-8		C9H28N3O15P5	Scale Inhibitor	0.414042	159
Dipropylene glycol monomethyl ether CAS_34590-94-8	$CH_3OC_3H_6OC_3H_6OH$	C7H16O3	Acid/Corrosion inhibitor	0.386894	66
Didecyldimethylammonium chloride CAS_7173-51-5		C22H48NCl	Biocide	0.349976	707
N,N-DIETHANOLOLEAMIDE CAS_93-83-4		C22H43NO3	Friction Reducer	0.308551	339
BENZALKONIUM CHLORIDE CAS_68424-85-1		C17H30NCl	Biocide	0.29212	769
Ethanol CAS_64-17-5		CH3CH2OH	Biocide	0.270841	748
Polyquaternium-33 CAS_69418-26-4		(C8H16ClNO2)x.(C3H5 NO)x	Friction Reducer	0.258788	397

Table 2—Ten ingredients most negatively correlated with gas productivity

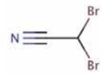
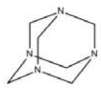
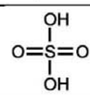
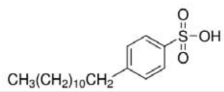
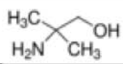
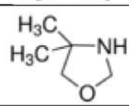
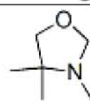
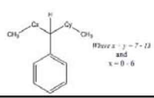
Chemical Name & CAS No.	Chemical structure	Chemical formula	Purpose	Efficacy factor	Occurances (1/3246)
Dibromoacetonitrile CAS_3252-43-5		Br2CHCN	Biocide	-0.07	536
Hexamethylenetetramine CAS_100-97-0		C6H12N4	Acid/Corrosion inhibitor	-0.07	143
Sulfuric acid CAS_7664-93-9		H2SO4	Non-Emulsifier/Breaker	-0.08	307 (14+293)
Dodecylbenzenesulfonic acid CAS_27176-87-0		C12H25C6H4SO3H	Non-Emulsifier	-0.09	407
Sodium nitrate CAS_7631-99-4	$NaNO_3$	NaNO3	Nitrate Reducing Bacteria	-0.10	270
β-Aminoisobutyl alcohol CAS_124-68-5		C4H11NO	Biocide	-0.11	81
4,4-DIMETHYLOXAZOLIDINE CAS_51200-87-4		C5H11NO	Biocide	-0.11	81
3,4,4-trimethyl oxazolidine CAS_75673-43-7		C6H13NO	Biocide	-0.11	81
Benzene, C10-16-alkyl derivatives CAS_68648-87-3		C19H32	Non-Emulsifier	-0.17	293
Sulfur Dioxide CAS_7446-9-5	SO2	SO2	Non-Emulsifier	-0.17	293

Figure 2 and Table 1 list the top 10 chemicals that are most conducive to gas production. The empirical notion that for more production, more proppant is needed, or "pump until it screens out", is corroborated by the data-based learning as show in Figure 2, where sand and water have the highest positive efficacy factor with gas production.

Lesser known is the learning that ammonium chloride (NH4Cl), a common fertilizer, is also strongly beneficial to gas production. It is often used in tandem with Diethylenetriaminepentakis (methylphosphonic acid) (DTPMP), Dipropylene glycol monomethyl ether (DPGME), and N,N-Diethanololeamide (DEA). The compound of these four ingredients (NH4Cl, DTPMP, DPGME, and DEA) has intended purpose of scale inhibitor, corrosion inhibitor and friction reducer.

Also learned is that a few biocides are particularly conducive to gas production, such as Didecyldimethylammonium chloride (DDAC). DDAC is often used in tandem with Ethanol, Glutaraldehyde, Benzalkonium chloride (BKC), and Poly(acrylic acid sodium salt) (PAAS).

Similarly, the top 10 chemicals that are most negatively related to gas production are listed in Figure 3 and Table 2. It is learned that Benzene, C10-16-alkyl derivatives (BAD) may function as non-emulsifier, but among the 326 ingredients it most negatively impacts gas production from the group of 3126 wells. It is used in tandem with small amounts of sulfur dioxide, Dodecylbenzenesulfonic acid (DBSA) and Calcium nitrate. These ingredients and their compounds should be avoided in fracturing fluid formulation, as the data shows.

Also detrimental to gas production are a group of biocides: β-Aminoisobutyl alcohol, 4,4-DIMETHYLOXAZOLIDINE and 3,4,4-trimethyl oxazolidine. These three biocides are used hand-in-hand in the same 81 wells.

Based on the model, gas production of each of the 3126 wells is predicted against its actual production, as shown in Figure 4 (production are normalized). The overall prediction error is within 30%.

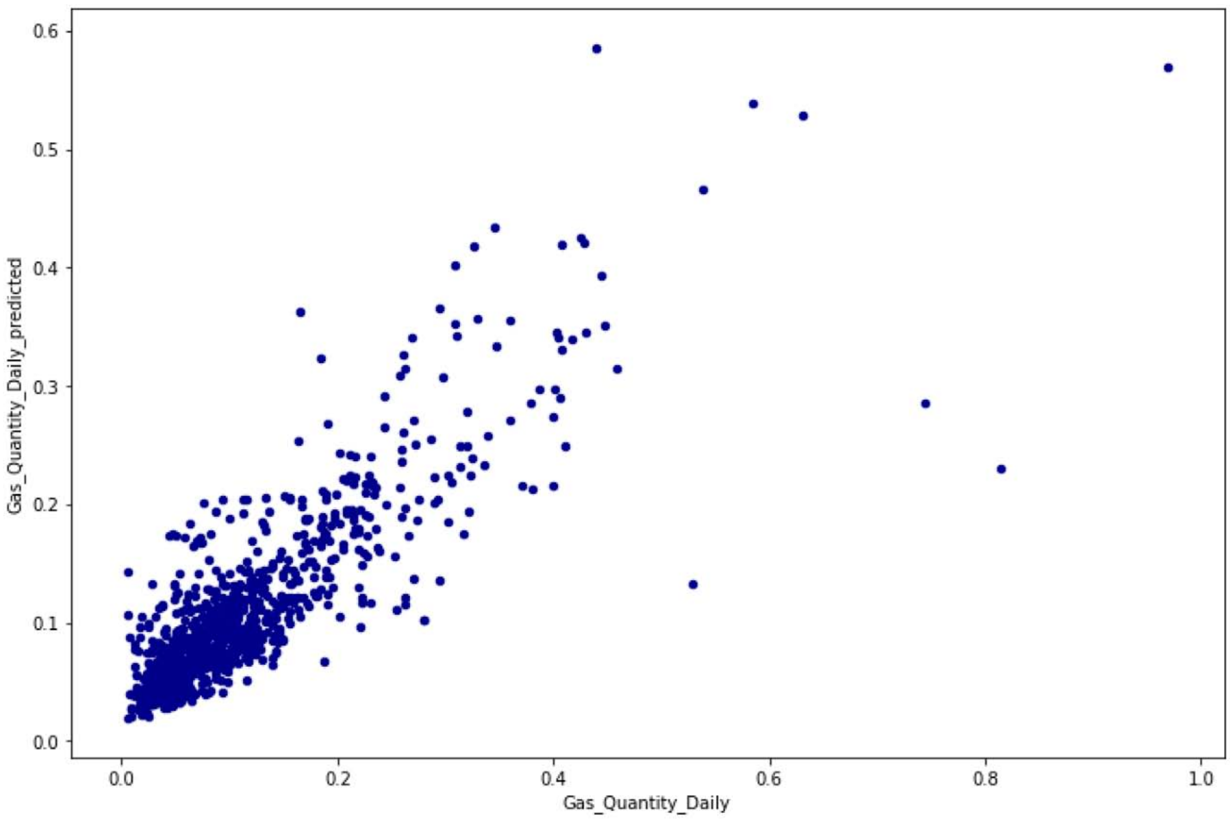


Figure 4—Predicted gas production vs actual gas production (normalized values)

Interpretation

The findings in section 2.4 are learned from FracFocus and production data of the 3126 wells by algorithms. For a scientist, the data mining framework would not be complete absent of understanding of the chemical mechanism or physical models behind the findings.

On the first look of the list in Table 2, sulfuric acid will generate sulfate ions, and sulfur dioxide may also be oxidized to form sulfate ions during fracturing operations. Since the sulfate ion is food for unwanted sulfate reducing bacteria, it could be one mechanism that sulfuric acid and sulfur dioxide appear in the top 10 ingredients most negatively correlated with gas productivity.

Another mechanism for the disadvantages caused by sulfate or sulfite is the possibility of their incompatibility with Ba2+ ions connate in formation waters in Pennsylvania (Figure 5). The USGS has published a geochemical database of produced waters (Blondes 2017), which contains water chemistry data of 115,000 water samples, out of which 423 are from Marcellus shale gas wells in Pennsylvania. About 250 water samples out of the 423 had Barium ionic concentration greater than 50 mg/L (this subset of the database was compiled from various sources [Kresse 2013, Osborn 2010, Cluff 2014, Shih 2015, Chapman 2012, Hayes 2009, Akob 2015, Engle 2011, Engle 2015] by USGS. The following figure shows the well locations where these 250 produced water samples were collected. Note that 56 of the 250 have Barium concentration in the range of 50-500 mg/L, 144 in the range of 500-5000 mg/L, and 39 in the range of

5000-25000 mg/L, and some samples apparently were collected from the same well, so there are overlaps among the dots in Figure 5.

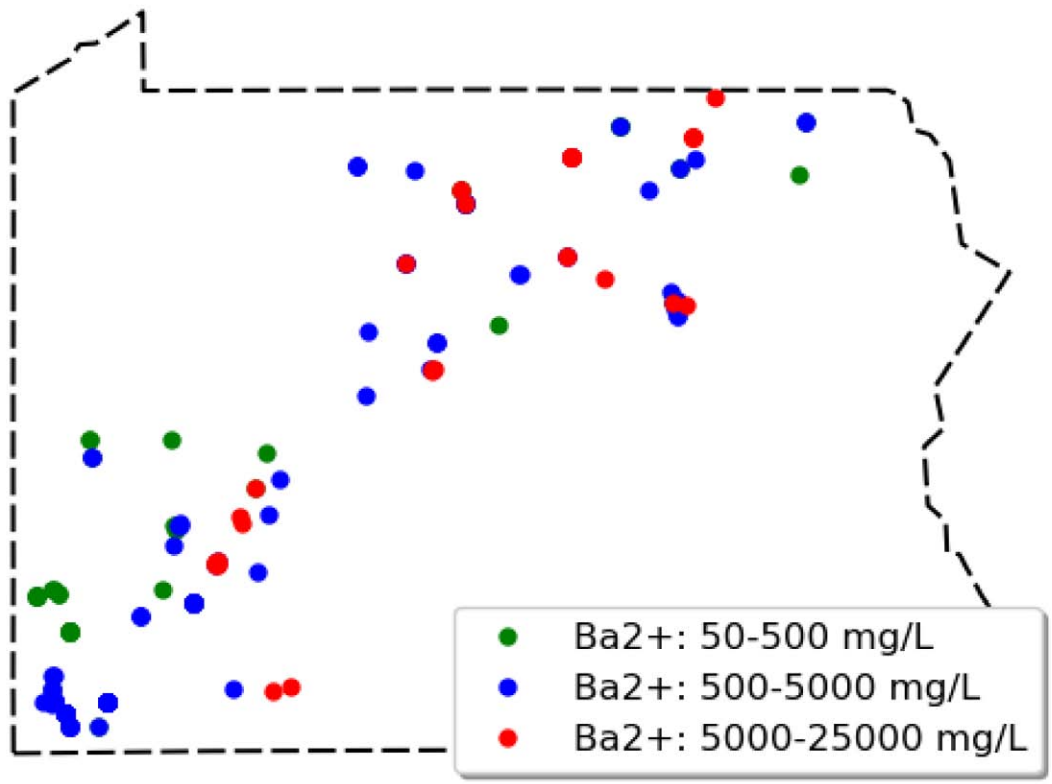
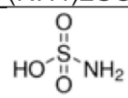


Figure 5—Well locations of water samples reported with high Ba2+ concentration

However, a closer examination at the dataset in Section 2.3 shows that sulfur dioxide and sulfuric acid were only used at trace amounts (less than one lbs) as an additive to non-emulsifier Benzene, C10-16-alkyl derivatives (BAD) in the same 293 wells. And for the 14 wells that sulfuric acid was not associated with BAD, its quantity was also on the order of 10 to 20 lbs, unlikely to be the main driver for either significant sulfate bacteria growth or barium sulfate precipitation.

To further establish or exclude the Ba2+ possibility, a compilation of sulfides, sulfates and persulfates that appeared in the dataset for modeling is shown in Table 3. These sulfuric ion containing chemical ingredients all have gas production efficacy factors close to zero, meaning that they are neither beneficial nor detrimental to gas production. It is therefore determined that the Ba precipitation mechanism was not a concern for the 3126 wells modeled. Instead, chemical mechanism research should be focused on non-emulsifier Benzene, C10-16-alkyl derivatives (BAD).

Table 3—Sulfides, sulfates and persulfates that appeared in the dataset

Chemical Name & CAS No.	Chemical structure	Chemical formula	Purpose	Efficacy factor	Occurances (1/3246)
Sodium Persulfate CAS_7775-27-1	$Na_2S_2O_8$	Na2S2O8	Breaker	-0.02	180
Ammonium Persulfate CAS7727-54-0	$(NH_4)_2S_2O_8$	(NH4)2S2O8	Breaker	-0.02	441
Sodium Sulfate CAS_7757-82-6	Na2SO4	Na2SO4	Iron Control Agent	-0.01	186
Ammonium Sulfate CAS_7783-20-2	(NH4)2SO4	(NH4)2SO4	Friction Reducer	0.02	181
Sulfamic Acid CAS_5329-14-6		NH2SO3H	Friction Reducer	0.06	28

Nitrates have been used in fracturing fluids to promote growth of nitrate reducing bacteria (NRB) to crowd out the growth of unwanted sulfate reducing bacteria (SRB), and it has been claimed to be more effective in controlling sulfide corrosion than biocides killing SRB [Degner 2015]. Although nitrate treatment is maturing, it still has not been fully evaluated to establish clear criteria for implementation covering a wide range of different oil field conditions [Saudi Aramco J. Of Tech. Winter 2015].

For example, sodium nitrate is one of the top 10 most negative ingredients in Figure 3 and Table 2. It was used often with four other negative ingredients sulfur dioxide, sulfuric acid, BAD, and DBSA in Figure 3 and Table 2.

Another nitrate, Calcium nitrate (Ca(NO3)2), which was also used in conjunction with the same four negative ingredients, has a gas production efficacy factor of −0.05. Surprisingly, the hydrate form of calcium nitrate tetrahydrate (Ca(NO3)2-4H2O), which has a markedly positive gas production efficacy factor of +0.09, was mostly used along with four other ingredients sodium DL-lactate solution, KH2PO4, CH3COONa, 2-Amino-5-chlorobenzophenone. It is speculated that nitrates may be conducive to gas production, and calcium nitrate has higher ratio of nitrate ions than and can be more beneficial than sodium nitrate. But their positive effect on gas production may also be enhanced or compromised by the chemical ingredients associated with them. Choosing compatible chemical ingredients is crucial for nitrates to help increase gas production.

In the field, the selection of chemicals is often empirical since the geological context may be only partially understood, the fluid chemistry is complex, and/or completion designs need to be changed on the fly. Therefore, a fracturing fluid ingredient may or may not serve its intended purpose. For example, nitrates as corrosion inhibitor have contentious effectiveness with reports varying from beneficial in controlling corrosion to significantly increasing localized attacks and corrosion rates [Rizk 2006, AI-EES 2012]. Learned from the FracFocus and production data, the efficacy factors of ingredients could be used to stop the guess work of which ingredients are compatible and conducive to production while others are incompatible and detrimental to production.

Validation

In order to cross check the modeling results in Section 2.4, we pick two groups of biocide ingredients and compare the gas production with the ingredients from each group:

a. Didecyldimethylammonium chloride which was used in 707 wells (Table 1);

b. β-Aminoisobutyl alcohol, 4,4-DIMETHYLOXAZOLIDINE and 3,4,4-trimethyl oxazolidine which were used together in one product in the same 81 wells (Table 2).

Two sample t-test independent of the modeling algorithm in Section 2.4 is performed to predict the gas production if (a) were to replace (b) in the 81 wells. The result shows that:
t-statistic = 8.32,
p-value = 4.4 e-16

Since the p-value is infinitesimally small, we can safely say that the production enhancement would be significant. The biocide ingredient in group (a) would have helped the 81 wells produce 310% more gas in replacement of the biocide ingredients in group (b), which is in agreement with their big contrast in efficacy factors (0.35 for (a) and −0.11 for (b)).

Conclusions

A framework of big data analytics is developed to measure the efficacy factor of fracturing fluid ingredients in terms their effectiveness on well productivity, based on FracFocus and well production databases. Such efficacy factors could serve as justification for chemical product approvals and denials.

As a useful demonstration, chemical ingredients that are conducive to production of wells with Marcellus shale geology are quantitatively differentiated those that negatively impact gas productivity. The specific efficacy factors may not be directly applicable in other fields, but the framework of data analysis can be easily applied.

The data analytics framework helps providing leads in understanding the intricate chemical and physical processes of fracturing fluids. It points the direction to the causality - those kinds of cause-effect relationships – between ingredient and productivity straight from real-world data.

Each well is a geophysical experiment. Compared with fracturing fluid lab test that still needs to be optimized in the field, the data analytics framework learns hidden connections from field data, which is the ultimate experiment, and reduces or stops the guesswork.

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