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Modeling and Simulation for Estimating Injection Dose Rate of a Hydrogen Sulphide Scavenger for Treating Natural Gas



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Abstract

A common issue in many oil and gas fields is the presence of hydrogen sulphide H₂S in the hydrocarbon fluids. Unwanted contamination of H₂S poses several risks to public health and the environment. It is caustic, offensive, and corrosive. As a result, the industry has long been in need of a technique that can reliably remove H₂S from natural gas, or at least lower its level during production, storage, or processing to meet safety and product specification criteria. A common method for eliminating or lowering the concentration of H₂S in hydrocarbon production fluids is to inject an H₂S scavenger into the hydrocarbon stream. The Egyptian Petroleum Research Institute (EPRI) produces EPRI H₂S scavenger, which is one of their compounds. This injection dosage rate is calculated statistically using modeling and simulation of a Zohr Gas field in the Mediterranean Sea as a case study. The project entails the construction of a gas field Zohr, Egypt, with a daily capacity of 850 billion standard cubic meters. The H₂S inlet concentration, pipe length, diameter, pressure, and gas flow rate all play a role in determining the ideal H₂S scavenger injection dosage rate. Using the software application Lingo, the optimization results are achieved for various values of these parameters. In general, increasing the diameter of the pipe and raising the intake H₂S concentration increases the optimal values of the H₂S scavenger injection dosage rate for hydrogen sulphide scavenging, whereas increasing the length of the pipe, gas flow rate, and pressure decreases them.

Keywords: Modeling; simulation; H₂S Removal; H₂S Scavenger; injection dose rate.

1. Introduction

The economic value of produced hydrocarbons and production methods are significantly impacted by the chemical hydrogen sulphide (H₂S) [1, 2]. It is a weak acid that corrodes metals and dissolves in some solvents, including water, alcohol, and oils [3-5]. It is exceedingly poisonous to human and animal life and may cause drill pipe and tubular products to shatter, making it dangerous to people on the surface [6-8]. Fluids in permeable formations of natural gas wells with a high hydrogen sulphide concentration, natural gas typically contains 0.01-0.4% sulphur by weight [9, 10].

As a result, removing H₂S from formation or flow back fluids has become a requirement. Using H₂S scavenger is one of the numerous strategies for removing H₂S [11-14]. Scavengers for hydrogen sulphide are compounds that react positively with H₂S gas to remove it and generate environmentally benign products, depending on the kind and content of the scavenger as well as the reaction circumstances [15-19]. Some scavengers, such as metal-based scavengers, create solids, whereas others, such as triazines, yield soluble compounds [13, 14, 20]. As a result, selecting the right scavenger for a certain recipe is just as important as its function. During effective stimulation treatments, the outcomes of the interaction between H₂S and a scavenger should not affect the formation [21-24].

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The H₂S scavengers are typically designed to react successfully under a variety of in-situ situations [11, 25]. Triazine-based scavengers, for example, are developed for neutral-high pH circumstances, whereas aldehyde-based scavengers are suited for low pH situations; nevertheless, the reaction products of these scavengers with H₂S may cause formation damage [26, 27]. Scavengers based on triazine have mostly been employed in stimulation therapies to eliminate H₂S from flowing back fluids. The efficacy of triazine-based H₂S scavengers during stimulation treatments is affected by factors such as pH, temperature, and exposure period [28-30]. Triazinebased H₂S scavengers' interaction with H₂S can also be influenced by other variables, such as the H₂S/scavenger stoichiometry. For instance, raising pH from 0 to 7 increased scavenging capacity on average by 176%. The hydrolysis rate, which rises with acidity, is the cause of this [31].

Any form of scavenger that is used in manufacturing activities must adhere to strict guidelines since the security of the workers and the machinery rely on it. The following qualities are essential for a good scavenger [32-35]:

Its reaction with sulfuric acid needs to be thorough, quick, and predictable. Under all mud circumstances, the reactive product(s) generated should continue to be inert. Scavenging should be supported by a number of the system's chemical and physical characteristics.

Even at high temperatures, the system's overall performance, including mud archaeology, filtration, and cake quality, shouldn't be negatively impacted by excessive scavenging. This work examines modeling and simulation for rate calculation of H₂S scavenger injection dose to remove H₂S from oil and gas fields.

2. Experimental

2.1. Estimation of Injection Dose Rate

For calculating the absorption of H_2S from petroleum production, the following simplified equation was used to determine the average ideal mass transfer coefficient, which is given as values. The rate equation is used to estimate the amount transmitted [36]:

$$\frac{dy_{H_2S}}{dz} = \frac{K_g a P y_{H_2S}}{G_V} \tag{1}$$

Where y_{H2S} is the mole fraction of H_2S in the gas phase; G_V is molar gas velocity, mol/m²s; Z is tube length, ft; K_g is overall mass transfer coefficient, mol/m² s bar; a is an interfacial area, m²/m³; and P is pressure, bar. The pressure and molar gas velocity will vary along the path. With the same rate of lift gas injection and flow rates in an oil well, the rate constant (Kga) is determined using field data of H₂S concentration injection of scavenger solution. Without introducing any H₂S scavenger, mass balance was used to determine the H₂S concentration at the entry was calculated using the operational H₂S concentration that was obtained while injecting a known quantity of an H₂S scavenger solution at a specified lift gas flow rate.

$$\frac{K_g a P}{G_v} Z = \ln \frac{y_{in}}{y_{out}}$$
(2)

Where

 K_{g} = overall ideal mass transfer coefficient, mol/m² s bar

a = interfacial area, m^2/m^3

 $G_v = gas molar mass velocity, lbmol/(hr m²)$

P = Pressure, bar, Z= Pipe length, m $y_{in}, y_{out} = inlet$ and outlet H₂S concentration ppmv.

This equation is developed using an ideal model in which the equilibrium vapour pressure of H_2S is 0 and the values remain constant throughout the pipe's length. However, as the stoichiometric limit of the scavenging agent is reached, test field data reveal that the value does vary (it lowers) along the length of the pipe, and the vapor pressure of H_2S eventually rises.

Despite the idealized model short comings, equation (3) offer saverage value estimations and may be used to successfully anticipate H₂S removal over a wide variety of flow conditions. Equation (4) was used to obtain the average real mass transfer coefficients for various pipe lengths.

The average values were derived using the input H₂S concentration and the H₂S measured downstream at various pipe lengths of the injection site. To get the best fitting coefficients, the following equation was regressed using a typical statistical method:

$$K_{ga} = C_{1} G_{v}^{C_{2}} R_{j}^{C_{3}} D^{C_{4}}$$
 (3)

Where:-

 K_{ga} = Coefficient of mass transfer, 1 bmol/ (hr m³ bar)

D = diameter of pipe, inches

 $R_{\rm J}$ = Dose injection rate of H_2S scavenger, gallons/ MMSCF

 $G_V = gas molar mass velocity, 1 bmol / (hr m²)$

 C_1 , C_2 , C_3 , C_4 = Regression Coefficients Constants.

From equations (1) and (2) then the finally empirical equation to obtain the optimum dose injection rate of H_2S scavenger using the software program Lingo [37].

$$R_{j} = \frac{F^{*10}}{24} \left[\frac{\ln \frac{y_{in}}{y_{out}} G_{v}}{C_{1} G_{v}^{C_{2}} D^{C_{4}} PZ} \right]^{1/C_{3}}$$
(4)

Where:-

 $R_{\rm j}$ = Dose injection rate of H_2S scavenger, gallons/ MMscf

F = Gas flow rate MMSCFD

In the 3,752 km² Shorouk Block, which is part of Egypt's Exclusive Economic Zone (EEZ), in the Mediterranean Sea, is where our case study, the Zohr Gas field, is situated. The Egyptian Natural Gas Holding Company (EGAS) will begin construction on the 850 billion standard cubic meters of gas per day Zohr gas field as part of the project in February 2016. The deep water gas field began production in 2017 and achieved its maximum output in 2020. The daily MMSCFD flow output, water cut BS & W%, temperature C, wellhead pressure psi, and other wells field data from an existing natural gas well in the Zohr field in Egypt are provided in Table 1.

Table 1Zohr natural gas field productionconditions

flow rate MMSCFD	350
Pressure, bar	80
Temperature, ⁰ C	40
line diameter, inch	24
line length, m	985
H ₂ S concentration inlet	200-1000 PPM in gas
H ₂ S concentration after chemical treatment	Required to be treated to 4 ppm

3. Results and Discussion

According to the empirical equation 1, the optimal hydrogen sulphide scavenger injection dosage rate depends on the following variables: diameter of the pipe, pipe length, gas flow rate, inlet concentration of H_2S , and pressure.

3.1. The H₂S Scavenger Injection Dose Rate Optimum Value at Different Pressures

Figure 1 shows the H_2S scavenger injection dose rate optimum values to be treated to 10 ppm at different inlet H_2S concentrations 200, 400, 600, 800, 1000 ppm and at different pressures, 20, 40, 60, 80, and 100 bar respectively and gas flow rate is 350 MMSCFD, pipe diameter 24 inches and pipe length 1000 m. In general, increasing pressure from turbulence and increasing gas velocity will result in better mixing between the scavenger and the crude, lowering the ideal values of the H_2S scavenger injection dosage rate to be treated to 4 ppm.



3.2. The H₂S Scavenger Injection Dose Rate Optimum values at Different Pipe Diameters

Figure 2 shows the H₂S scavenger injection dose rate optimum values to be treated at different inlet H₂S concentrations 200, 400, 600, 800, and 1000 ppm and at different pipe diameter values 16, 20, 22, 24, and 28 inch, respectively and gas flow rate 350 MMSCFD, pressure 80 bar and pipe length 1000 m. Increasing the pipe diameter often led to an increase in the optimal value of the H₂S scavenger injection dosage rate because it reduced turbulence and gas

velocity, which led to a lack of effective mixing between the natural gas and the scavenger.



3.3 The H₂S Scavenger Injection Dose Rate Optimum Values at Different Pipe Lengths

Figure 3 shows the H_2S scavenger injection dose rate optimum values to be treated at different inlet H_2S concentrations 200, 400, 600, 800, and 1000 ppm at different pipe length values 164,328, 492, 656, 820, and 985 m, respectively, gas flow rate 350 MMSCFD, pipe diameter 24 inches, pressure 80 bar. The optimal H_2S scavenger injection dosage rate will often decrease as pipe length increases due to an increase in response retention time.



3.4. The dose injection rates of H₂S scavenger optimum values at different gas flow rates, (MMSCFD)

Figure 4 shows the dose injection rate of H₂S scavenger optimum values to be treated at different inlet H₂S concentrations 200, 400, 600, 800, and 1000 ppm at different gas flow rates 250, 300, 350, 400, and 450 MMSCFD, respectively and pipe length 1000 m, pipe diameter 24 inches and pressure 80 bar. Due to a rise in response retention time, the ideal values of H₂S scavenger injection dosage rates are often reduced by increasing gas molar mass velocity.



350

4. Conclusion

One of the Egyptian natural gas firms researched the modeling and simulation of the scavenging process of hydrogen sulphide from the output of the Zohr natural gas field. H₂S levels in the natural gas mixture initially vary from 200 to 1000 ppmv, but it is required to lower them to at least 10 ppmv before processing. The Egyptian Petroleum Research Institute's (EPRI) H₂S scavenger chemical is used to do this process. The pipe diameter, pipe length, gas flow rate, pressure, and temperature all affect how much scavenger is injected. It investigated how these factors affected the rate of H₂S scavenger injection. Within the parameters that were examined, it was discovered that the following conclusions could be made:-

The scavenging process is negatively impacted by increasing pipe diameter due to decreased gas velocity and turbulence, which results in poor mixing of the scavenger and flow. The scavenging procedure is impacted by the length of the pipe. H₂S scavenger injection dosage rate falls as pipe length grows as a result of longer contact times.

The length of the pipe should be increased to allow the scavenger ample time to react with the H_2S present in the natural gas. The H_2S scavenger injection dosage rate rises when gas flow rate is increased while maintaining a fixed pipe diameter. The gas flow rate barely affects the rate of H_2S scavenger injection.

The H₂S scavenger injection dosage rate reduces when pressure is raised. The pressure has a significant impact. The ideal temperature range is between 55 and 70 °C since this range of temperatures is sufficient to cause the dissolved H₂S in water and natural gas to enter the gas phase.

The estimation of the chemical scavengers' injection rates was done after modeling and simulating the hydrogen sulphide concentration profiles for various field data under various situations. The computation's findings are consistent with the actual injection dosage rate during the production of the zohr natural gas fields.

Conflict of Interest

"There are no conflicts to declare".

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