Numerical calculation and analysis on phase behavior of fireflood exhaust from HQ-1 well in Xinjiang oilfield

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Abstract. For designing a reinjection system of fireflood exhaust, phase calculation and analysis are the most fundamental things. Aspen Hysys and FEPE which was developed with our own intellectual property rights were employed to study the phase envelope of fireflood exhaust from HQ-1 well. After comparing the applicability of the software adopted, the rule of phase behavior and affecting factors were summarized. The result shows that the composition and phase envelope of fireflood exhaust are dramatically different with that of natural gas. Envelope Utility, a tool which is commonly used to produce fluid phase envelope in Aspen Hysys, makes fault in generating that of wet fireflood exhaust. By contrast, FEPE can produce the dew point line for wet and water-free fireflood exhaust, showing batter applicability than Envelope Utility. The results also show that among the components, water content affects the dew point most seriously. There will exist liquid-vapor phase during rejection process, which will threaten the rejection safety. Thus, for safety’s sake, it is required to take prevention measures such as dehydration to avoid corrosion and other risks.

1. Introduction
In-situ combustion (fireflood) technology [¹] enhances the heavy oil recovery, and produces lots of fireflood exhaust meanwhile. With its further application on Chinese Shengli[², ³], Liaohe[⁴-⁶] and Xinjiang oilfield[⁷, ⁸], how to treat the fireflood exhaust becomes the critical role in the whole in-situ combustion strategy.

The fireflood exhaust mainly consists of N₂ and CO₂, and contains a small amount of CH₄、H₂S、O₂ and other components[⁹]. Discharging it into atmosphere directly will cause serious environmental pollution and irreparable waste of non-renewable resources[¹⁰]. Considering that the composition is similar to that of flue gas[¹¹], the idea of flue gas injection for EOR[¹²-¹⁵] can be employed. After being treated, the fireflood exhaust will be injected into other proper layers for EOR, which decreases greenhouse gases emission and fully uses fireflood resource simultaneously. This program is about to
be started in Xinjiang oilfield, CNPC, which can be seen as another efficient treatment process besides burning\cite{10, 16}, desulfuration\cite{17-20} and pressure swing adsorption\cite{17, 19-22}.

Phase analysis is the fundamental of any treatment process. The fireflood exhaust from HQ-1 Well of Xinjiang oilfield is selected to research the phase change during reinjection process in this paper, aiming at precisely describing its phase behavior character. Compared with commercial and experimental data, a civil-right software named FEPE is used to further study the law of phase change. The achievement can be the basic theory and engineering application platform for design and management of fireflood exhaust reinjection system.

2. Composition of Fireflood Exhaust to Be Injected

The composition of injected fireflood exhaust from HQ-1 well is showed in Table 1.

Table 1 Simulated composition of wet fireflood exhaust

| Component (mole%) | C₁ | C₂ | C₃ | C₄ | C₅ | CO₂ |
|------------------|----|----|----|----|----|-----|
| Fluctuation range | 1~8 | 0~0.5 | 0~0.3 | 0~0.4 | 0~0.2 | 10~16 |
| Component Content | H₂S | N₂ | H₂ | O₂ | CO | H₂O |
| Fluctuation range | 0.03~0.3 | 75~80 | 0~2 | 0~3 | 0~1 | 2.58 |

It can be seen from table 1 that the fireflood exhaust is mainly composed of nitrogen and carbon dioxide, a small amount of alkanes and oxygen and trace hydrogen sulphide. The composition character is similar to that of flue gas. This composition is used in the discussion studies below.

3. Phases Analysis of Fireflood Exhaust

3.1 Phase analysis by Envelope Utility in Hysys

As one of famous simulation software for chemical treatment in the word, Aspen Hysys can achieve many goals, such as analyzing phase behavior of fluids, designing chemical treatment factories, monitoring and optimizing equipment and so on. In the software, Envelope Utility can produce the phase envelope of specified fluid automatically, which has the priority to be used for studying the phase character of fireflood exhaust during reinjection process.
Figure 1. Phase envelope of wet fireflood exhaust using different EOS

Figure 1 illustrates the phase envelope of wet fireflood exhaust employing Envelope Utility with seven EOS. It can be seen that with the bubble point line missing, the envelope only consists of dew point line, and is dramatically different from that of conventional natural gas in shape. Extreme point exists for each dew point line. The tendency is similar to that of Du 66 block fireflood exhaust in Liaohe oilfield [20], CNPC, illustrating that, from various oilfields, there is a consistency in the phase envelope of the fireflood exhaust with N₂ and CO₂ as the main components.

The reinjection process consists of multistage compression, cooling, separation and so on. By comparing the reinjection parameter curve and the phase envelope, it can be deducted that there is no phase change during reinjection process, as shown in Figure 2.

Figure 2. Comparison of calculated dew points of wet fireflood exhaust with designed process parameter
However, it is found that in some cases, the vapor ratio calculated with Envelope Utility for wet fireflood exhaust goes contrary to that of phase equilibrium. Table 2 lists the difference of phase judgment between Envelope Utility and flash calculation at some specified conditions.

| No. | Working conditions | Whether there exists liquid phase | No. | Working conditions | Whether there exists liquid phase |
|-----|--------------------|----------------------------------|-----|--------------------|----------------------------------|
| 1   | 0.5MPa/50℃         | x                                | 7   | 5MPa/123℃          | x                                |
| 2   | 1.2MPa/50℃         | x                                | 8   | 5MPa/40℃           | x                                |
| 3   | 1.2MPa/150℃        | x                                | 9   | 10MPa/123℃         | x                                |
| 4   | 1.2MPa/5℃          | x                                | 10  | 10MPa/40℃          | x                                |
| 5   | 2.5MPa/90℃         | x                                | 11  | 20MPa/121℃         | x                                |
| 6   | 2.5MPa/40℃         | x                                | 12  | 20MPa/50℃          | x                                |

Meanwhile, it is also found that the dew point lines of fireflood exhaust in six water contents generated by Envelope Utility are basically consistent, as shown in Figure 3, which disobeys fundamental theory and may mislead the managers and researchers. Hence, employing the Envelope Utility in Hysys is not appropriate for studying the phase behavior of fireflood exhaust.

3.2 Phase analysis by point-to-point computation

Point-by-point computation with Hysys is carried out. That is, for a specified composition and pressure, vapor fraction is set to 1 and 0 to get the corresponding dew and bubble temperature, respectively. Figure 4 shows the dew point lines of wet fireflood exhaust made by point-by-point computation.

It can be seen from Figure 4 that the dew point line appears obvious different with Figure 1 to 3. For the same wet fireflood exhaust composition, pressure and EOS, Figure 4 shows higher dew temperature compared with that formed by Envelope Utility automatically. During reinjection process, two-phase region exists so that dehydration is necessary. However, the conclusion made by Envelope
Utility comes on the contrary that the reinjection parameters are all located in vapor phase region. It will mislead designing process and selecting equipment et al., threatening the safety of reinjection system.

![Figure 4 Dew point lines calculated by point-by-point computation](image)

We can conclude from the above calculation that when employing Hysys to study the phase envelope of fireflood exhaust, the method of point-by-point computation is more reasonable than using Envelope Utility automatically. But the former takes more manual labour. Meanwhile, because the phase envelope of fireflood exhaust with and without water content generated by Envelope Utility in Aspen Hysys seems little discrimination, it would mislead the designers, researchers and managers about detailed process program. Hence, for fireflood exhaust, it’s meaningful to develop a specialized professional phase and property simulation software which can not only compute the phase equilibrium and physical properties, but also discriminately show the phase envelope with and without water component.

4. Fireflood Exhaust Phase Equilibrium (FEPE) Software

4.1 Introduction to FEPE

On the basis of our independent intellectual property products named PK2018[23] - a computation software platform for oil and gas gathering and transportation, Fireflood Exhaust Phase Equilibrium (FEPE) is developed. PR[24] and NIST extension model[25-28] are included for selection. FEPE is able to achieve phase equilibrium and property prediction of fireflood exhaust, generating its phase envelope. The calculation result is presented in form of data sheet and curve, and can be output into Word or Excel directly.

4.2 Validation of FEPE

To verify the software, 5 representative fireflood exhaust samples (Table 3) are selected to compare the dew points calculated by FEPE with Hysys (point-by-point computation method) and corresponding experimental value. The result is showed in Table 3.

Table 3 Composition of tested fireflood exhaust

| No. | CH4 | C2H6 | C3H8 | C4+ | N2 | CO2 | O2 | H2 | H2S |
|-----|-----|------|------|-----|----|-----|----|----|-----|
|     |     |      |      |     |    |     |    |    |     |
Relative error and mean relative error are calculated with the following formula, the result as shown in Table 4.

\[
RE = \frac{\text{Experimental value} - \text{Calculated value}}{\text{Experimental value}} \times 100\% \quad (1)
\]

\[
MRE = \frac{1}{n} \sum_{i=1}^{n} (RE) \quad (2)
\]

Table 4 Mean relative error of FEPE and Aspen Hysys

| Sample number | MRE of Hysys | MRE of FEPE | Difference value |
|---------------|--------------|-------------|-----------------|
| 1             | 1.04%        | 0.78%       | -0.26%          |
| 2             | 0.98%        | 1.19%       | +0.21%          |
| 3             | 2.91%        | 2.02%       | -0.89%          |
| 4             | 1.45%        | 1.29%       | -0.16%          |
| 5             | 1.81%        | 1.91%       | +0.10%          |
It can be seen from Figure 5 to Figure 9 that for 5 water-free fireflood exhausts, the tendency of dew points calculated with FEPE and Hysys keeps consistent with experimental data. Meanwhile, the accuracy is familiar, total mean relative error of FEPE being 0.2% lower than Aspen Hysys for the 5 samples.

Among the calculation results, some pressure has no corresponding dew temperature, which reflects non-convergence of numerical solution at those conditions. Define the failure rate as the percentage of data points that do not converge. Hence, it can be another key indicator to determine the performance of simulation software. The failure rates of FEPE and Hysys are shown in Table 5.

| No. | Total number of points | Hysys | | FPE |
|-----|------------------------|-------|-----|-----|
|     | Number of non-         | Failure rate | Number of non- | Failure rate |
|     | convergence points    |               | convergence points |               |
| 1   | 63                     | 15           | 23.81%         | 3             | 4.76%         |
| 2   | 64                     | 14           | 21.88%         | 7             | 10.94%        |
| 3   | 45                     | 16           | 35.56%         | 0             | 0             |
| 4   | 48                     | 16           | 33.33%         | 0             | 0             |
| 5   | 60                     | 12           | 20.00%         | 4             | 6.67%         |

Table 5 shows that FEPE self-developed has much lower failure rate than Aspen Hysys for the tested samples, demonstrating its better adaption for studying the phase behavior of fireflood exhaust.

Figure 11 illustrates the dew point line made by FEPE automatically for water-free and wet fireflood exhaust, respectively. Combining the designed process parameter, it can be easily inferred that dehydration of fireflood exhaust is required for preventing corrosion and other hazard situation due to the existence of liquid-vapor phase region during reinjection process.
In conclusion, for water-free fireflood exhaust, FEPE has the consistent trend and accuracy with Aspen Hysys. However, for wet fireflood exhaust, the dew point line automatically generated with Envelope Utility in Aspen Hysys appears little difference with that of water-free gas. This neither obeys the common sense nor the result calculated in the point-by-point method with the same software. By contrast, the difference in dew point line between water-free and wet fireflood exhaust produced by FEPE is much obvious. Hence, it is acceptable that FEPE is more suitable for studying the phase envelope of wet and water-free fireflood exhaust.

5. Case Analysis
Owing to that the composition will fluctuate within a certain range in Table 2, FEPE is applied to study the cases when C₁, CO₂, N₂, H₂S and O₂ reach their top and bottom content limitation. Meanwhile, assuming different water contents, its influence on the dew point line is studied, too. The result is shown as Figure 11 to 12.

It can be seen from the results that the water content is the most significant influence on the dew point of fireflood exhaust. Hence, for safety, dehydration should be paid more attention during reinjection process.

Figure 10 Comparison of calculated dew points of water-free and wet fireflood exhaust using FEPE with designed process parameter

![Figure 10](image)

Figure 11 dew point lines of multi cases

![Figure 11](image)

Figure 12 Dew point lines of fireflood exhaust for different water content

![Figure 12](image)
6. Conclusions

(1) The fireflood exhaust mainly consists of N₂ and CO₂, and contains a small amount of CH₄, H₂S, O₂ and other gases. In use of the flu gas flooding, injecting it into proper layers for EOR of heavy oil is another effective and energy saving method.

(2) The phase envelope of fireflood exhaust is different from that of conventional natural gas. Dew point lines of wet and water-free fireflood exhaust automatically generated with Envelope Utility in Aspen Hysys almost coincide, which disobeys fundamental theory and actual situation.

(3) The software named FEPE is developed for calculating the properties and phase equilibrium of fireflood exhaust. Compared with experimental data, FEPE has slightly higher accuracy and much less failure rate than Hysys. In addition, FEPE can generate the dew point lines of fireflood exhaust with and without water content, being suitable for studying the injection process.

(4) By the comprehensive analysis of designed process parameter and dew point line, it can be deducted that vapor-liquid phase will appear during injection process. So prevention measures, dehydration for example, should be taken in advance.

(5) Dew point lines of fireflood exhaust in the multi cases of different C₁, CO₂, N₂, H₂S, O₂, H₂O are calculated with FEPE. Among them, the content of H₂O plays the most significant effect.

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