Control effect of fracture system on fluid migration, chemical reaction, and carbon dioxide storage

Leilei Yang1,2, Guo Wei1, Weiquan Zhao1, Jing Hu1, Guangyou Zhu3, Qi Liu1

1. China University of Petroleum (Beijing), Beijing, China
2. State Key Laboratory of Petroleum Resource and Prospecting, China University of Petroleum (Beijing), Beijing 102249, China
3. Research Institute of petroleum exploration and development, Beijing, China

Corresponding author:
Name: Leilei Yang
Email: yangleilei@cup.edu.cn

Abstract. Carbon dioxide (CO₂) injection alters a reservoir’s original equilibrium, leading to gas–liquid–solid reactions within the reservoir, resulting in mineral dissolution and precipitation affecting the reservoir’s physical properties. Because of their good permeability, faults are critical in fluid dredging and dominant channel formation. The characteristics of faults, including their width and strata length, directly affect the path, distance, and range of fluid migration and exert further control on the trend of water–rock–gas geochemical reactions. This study focused on the control effect of the fracture system on the migration, reaction, and storage of supercritical CO₂. The faulted Cretaceous reservoir in the Kela-2 gas field of the Tarim Basin was selected as the study formation, and 10 heterogeneous profile models were established using multiphase-flow, solute-transport numerical simulation. The differences in fluid migration and reaction ranges under different fracture lengths, fracture widths, fracture physical properties, and CO₂ injection rate conditions were examined. The real-time changes in profile porosity were quantitatively determined, and the control effect of the fracture system on reservoir development was analyzed. The results showed that CO₂ fluid entering the formation migrates primarily along the fault. Under the condition of a wider fracture, the fracture’s fluid accumulation and reaction range increase, the degree of acidification is weak, and the ultimate porosity increase is small. When the fracture extends into the reservoir over a greater distance, fluid migrates over a greater distance, and the effect on both sides of the fracture is weak because of less fluid accumulation. Similarly, a higher injection rate causes a longer migration, producing a thin and long injection region similar to that of a long fracture. Better fracture properties result in a more obvious dredging effect. When the fracture’s permeability is insufficient, the injected fluid accumulates at the bottom of the fault, and eventually, only the porosity at the base of the fault changes significantly. In conclusion, the fracture system plays a very
important role in controlling fluid migration, reaction, and reservoir development through induced reactions, and different fracture conditions lead to different reservoir development conditions.

Keywords: Fault system. Carbon dioxide. Fluid migration. Geochemical reaction. Reservoir development

1. Introduction

Carbon dioxide (CO2), whether it exists as natural gas in a reservoir, is buried underground as a greenhouse gas or is injected artificially into a reservoir to exploit groundwater, geothermal water, or oil and gas. It destroys the reservoir or wellbore system’s original balance, causing physical and chemical reactions between fluid and rock. In a fractured reservoir, CO2 enters the formation as an acidifying fluid, causing mineral dissolution and precipitation, ultimately changing the reservoir’s physical properties. Because of the good permeability faults provide, they are critical in fluid diversion via dominant channel formation.

After faults form, reservoir fluids, such as groundwater and atmospheric freshwater, also migrate along them, react with the formation, and alter its porosity and permeability conditions (Wu, 2011; Luo, 2018). When the scale of the faulting is larger, the reservoir becomes more developed (Zhuang, 2017). Wang (2021) proposed that the reservoir, fluid, and fractures were factors exerting mutual control and influence. Under the action of tectonics, fractures initially form in the formation and are reformed via dissolution and alteration by internal fluids. Karst water might infiltrate downward along the fracture direction, reforming the reservoir. Simultaneously, fractures make the surrounding strata fragile, leading to the upwelling of deep hydrothermal fluids. This process results in further dissolution and transformation of fractures, and the surrounding strata become fractured, vuggy system reservoirs with various spatial structures. When conceptualizing fractures’ guidance of fluids, the fractures are presumed to be in an active stage. The width of faults and the length of the strata cut directly affect the path, distance, and range of fluid migration, controlling the trend of fluid–mineral geochemical reactions. Thus, controlling the fault system over supercritical CO2 migration and reaction and reservoir development under different fault widths, lengths, porosities, and injection rates, must be examined.

Existing oil and gas exploration data confirm that the Kelasu structural belt in the Kuqa Depression of the Tarim Basin is characterized by strong thrust–fold deformation. Regional seismic profiles also show obvious stratification and vertical superpositioning of structural deformation. Additionally, faults are present in the Cretaceous strata of the Kela-2 gas field. During diagenesis, along with the injection associated with oil and gas, a large number of acidic fluids enter the strata, causing mineral dissolution or precipitation, changing the physical properties of the strata. Faults play a guiding role, and their widths and lengths of their cuts into strata directly affect the trend of fluid–mineral reactions.

In this study, the Cretaceous strata of the Kela-2 gas field in the Tarim Basin, China, were selected as the research object. By considering the differences in fluid migration and reaction range under different fracture lengths, fracture widths, fracture physical properties, and CO2 fluid injection rates, 12 heterogeneous profile models were established using a numerical simulation program of multiphase-flow and multicomponent reaction migration to analyze the variation laws of porosity, minerals, and
fluids in reservoirs under various conditions and the control effect of the fracture system on reservoir development.

2. Overview of the study area

The Tarim Basin is located in the southern Xinjiang Uygur Autonomous Region, which is the largest inland basin in China (Fig 1). The Kuqa Depression is located in the northern Tarim Basin between the Tabei Uplift and the South Tianshan Orogenic Belt (Han, 2005). The study area has rich oil and gas resources and complex formation conditions. The Kela-2 super-large gas field is located in the Kela linear anticline belt in the northern Kuqa Depression. The main gas-producing layers are the Lower Cretaceous Bashijiqike (K1bs) and Paleogene Kumglimu Formation sandstones. The caprock, which is closed, is the salt rock of the Paleogene Kumglimu Group (Chu, 2014). The field is an ultra-high voltage, super-high yield, super-high abundance, and super-large integrated high-quality natural gas field.

![Fig 1 Structure units of the Kuqa Depression (modified from the Petro China Project Report, 2008)](image)

3. Model establishment

3.1. Model software

This study used TOUGHREACT simulation software. In 1998, based on TOUGH2 software, Xu Tianfu and others improved fluid–chemical coupling to create a relatively perfect nonisothermal, multiphase fluid reaction geochemical migration simulation software (Yang, 2015). It can simulate the temperature, fluids, multicomponent solute migration, and geochemical processes in different dimensions of pore or fracture medium during reservoir diagenesis in a saturated or unsaturated medium to simulate chemical reactions during diagenesis and analyze the reaction rules of mineral cementation, dissolution, and metasomatism and the transformation relationships among them (Xu, 2006).

3.2. Model concept

In this study, the Cretaceous strata in the Kela-2 gas field, with a burial depth of 3400–3500 m and an average thickness of 100 m, was used to establish the two-dimensional model. The fault dip angle was 14°, and the X-direction length was 500 m. The fault model was divided into 62 grids. Each fault grid was set to 4 m, and the other grids were divided at a constant spacing of 12 m. The Z-direction...
distance was 100 m, divided into 40 grids. The fault was encrypted, and each grid was 1 m. The others were divided with a constant spacing of 6 m. The width of the Y-direction was 4 m. The model contained 2480 grids (Fig 2).

![Fig 2 Diagram of fracture injection 2-D model](image)

### 3.3. Model scheme

Twelve sets of models (cases 1–12) were set up for the reservoir. Cases 1 and 9 were set up for fracture conditions. Cases 1, 3, and 4 were established for comparison, with fault widths of 4, 8, and 10 m, respectively. Cases 1, 2, 10, 11, and 12 were set up for analyzing reservoir porosity and permeability conditions (0.3 and $1 \times 10^{-11}$, 0.2 and $1 \times 10^{-12}$, 0.4 and $1 \times 10^{-10}$, 0.2 and $1 \times 10^{-11}$, and 0.3 and $1 \times 10^{-10}$, respectively). The fault lengths in cases 1, 5, and 6 were 83 m, 100 m, and 40 m, respectively. Finally, cases 1, 7, and 8 were set up to compare fluid injection rates with injection flow rates of 1, 0.1, and 2 kg/s, respectively. Table 1 shows the parameter settings in the different schemes. In each model, carbonic acid was injected into the bottom of the fault for 20 years.

| Case | Fault porosity | Fault permeability ($m^2$) | Fault width (m) | Fault length (m) | Injection rates (kg/s) |
|------|----------------|----------------------------|-----------------|------------------|------------------------|
| 1    | 0.3            | $1 \times 10^{-11}$         | 4               | 83               | 1                      |
| 2    | 0.2            | $1 \times 10^{-11}$         | 4               | 83               | 1                      |
| 3    | 0.3            | $1 \times 10^{-11}$         | 8               | 83               | 1                      |
| 4    | 0.3            | $1 \times 10^{-11}$         | 10              | 83               | 1                      |
| 5    | 0.3            | $1 \times 10^{-11}$         | 4               | 100              | 1                      |
| 6    | 0.3            | $1 \times 10^{-11}$         | 4               | 40               | 1                      |
| 7    | 0.3            | $1 \times 10^{-11}$         | 4               | 83               | 0.1                    |
| 8    | 0.3            | $1 \times 10^{-11}$         | 4               | 83               | 2                      |
| 9    | 0.3            | $1 \times 10^{-11}$         | 0               | 83               | 1                      |
| 10   | 0.4            | $1 \times 10^{-10}$         | 4               | 83               | 1                      |
| 11   | 0.2            | $1 \times 10^{-11}$         | 4               | 83               | 1                      |
3.4. Initial conditions of the model

3.4.1. Initial formation physical properties

According to data acquired from Cretaceous samples from the Kela-2 gas field of the Tarim Basin, the porosity distribution range is 0.9%–23.36%. In the model, reservoir porosity and permeability were set to 0.16 and $1 \times 10^{-13}$, respectively. Using the actual formation temperature and pressure conditions and the local geothermal gradient (3°C/100 m), the pressure gradient was set to 2.4 bars/100 m, the initial roof temperature was set to 117°C, the pressure was set to 110 bars, the initial floor temperature was set to 120°C, and the floor pressure was set to 350 bars.

3.4.2. Initial formation water chemistry and mineral conditions.

The Cretaceous formation water of the Kela-2 gas field in the Tarim Basin was modeled as NaCl-type water with high salinity, low ionic strength, a pH of 5–6, and high Na⁺ and Cl⁻ contents. The model concentration was set to 1 mol/kg H₂O, the K⁺, Ca²⁺, Mg²⁺, HCO₃⁻, Fe²⁺, AlO₂⁻, and SO₄²⁻ contents were small. The initial water chemical composition in the basic model was in a balanced state with the rock minerals. Table 2 shows the specific settings of the water chemical composition and ion concentrations.

| Chemical composition | H⁺ | Ca²⁺ | Mg²⁺ | Na⁺ | K⁺ | HCO₃⁻ | SO₄²⁻ | Cl⁻ |
|----------------------|----|------|------|-----|----|-------|-------|-----|
| Ion concentration (mol/Kg H₂O) | $0.6801 \times 10^{-3}$ | $0.3559 \times 10^{-2}$ | $0.2098 \times 10^{-2}$ | $0.9949 \times 10^{-3}$ | $0.1262 \times 10^{-3}$ | $0.3926 \times 10^{-2}$ | $0.7653 \times 10^{-10}$ | $0.1000 \times 10^{1}$ |

3.4.3. Initial mineral conditions.

The Bashijiqike Formation can be divided into three lithologic sections. The interstitial material is mostly miscellaneous base and cement. The cement comprises dolomite, with small amounts of illite and chlorite. From the results and previous tests of the mineral composition and clastic components of the reservoir, Table 3 shows the initial mineral species and relative contents of the model.

| Mineral | Quartz | Calcite | Illite | Chlorite | Albite | Kaolinite | Smectite −Na | Smectite −Ca | Dolomite |
|---------|--------|---------|--------|----------|--------|-----------|--------------|--------------|---------|
| Volume  | 64.00  | 1.0     | 3.9    | 0.3      | 2.0    | 0.65      | 0.03         | 0.04         | 24.0    |
fraction (\%) 

4. Results and discussion

4.1. Fluid migration and chemical reaction

After carbonated fluid enters a reservoir, migration and reaction occur. After injections of CO_2-containing fluid, HCO_3^- increases greatly in the formation; feldspar minerals dissolve; carbonate minerals such as iron dolomite and calcite, as well as sodium aluminate, precipitate gradually; and kaolinite, illite, smectite, chlorite, and other clay minerals have different degrees of dissolution or precipitation at different locations depending on the fluid filling. The chemical equations of mineral dissolution, precipitation, and transformation include the following:

\begin{align*}
2\text{KAISi}_3\text{O}_8 + 2\text{H}^+ + 9\text{H}_2\text{O} & \rightarrow \text{Al}_2\text{Si}_3\text{O}_8(\text{OH})_4 + 2\text{K}^+ + 4\text{H}_4\text{SiO}_4, \quad (1) \\
\text{CaCO}_3 + \text{H}^+ & \leftrightarrow \text{Ca}^{2+} + \text{HCO}_3^-, \quad (2) \\
\text{CaMg(CO}_3)_2 + \text{H}^+ & \leftrightarrow \text{Ca}^{2+} + \text{Mg}^{2+} + \text{HCO}_3^-, \quad (3) \\
2\text{KAISi}_3\text{O}_8 + 2\text{NaAlSi}_3\text{O}_8 + \text{Ca}^{2+} + \text{CO}_2 + 4\text{H}_2\text{O} & \leftrightarrow 2\text{CaCO}_3 + 2\text{Al}_2\text{Si}_3\text{O}_8(\text{OH})_4 \\
& + 2\text{Na}^+ + 2\text{K}^+ + 8\text{SiO}_2, \quad (4) \\
\text{Ca(Fe}_{0.7}\text{Mg}_{0.3})(\text{CO}_3)_2 + 2\text{H}^+ & \leftrightarrow \text{Ca}^{2+} + 0.7 \text{Fe}^{3+} + 0.3 \text{Mg}^{2+} + 2 \text{HCO}_3^- . \quad (5)
\end{align*}

Because the initial potassium feldspar content was 0, no dissolution reaction of this mineral occurred, but albite was dissolved under the action of acidic fluid. A large amount of dolomite was dissolved in the injection diffusion area, a large amount of calcite was precipitated in the fluid diffusion plume, and a small amount of iron dolomite was generated in the fluid diffusion plume. A small amount of kaolinite was dissolved, chlorite was dissolved in the injection diffusion region but generated in the fluid diffusion plume because of an increase in the Fe^{2+} concentration in this region, and small amounts of smectite and diaspore were generated. A trace amount of quartz formed in the formation. The reservoir’s porosity increased. In case 9, the absence of a fracture spread the effect around the injection point and the development of greater porosity closer to the affected area’s center (Fig 3).
4.2. Control of fracture

The influence of fluid injection on reservoir porosity differs considerably under different fracture widths, lengths, and injection rates. The specific details of the analysis follow.

(1) Influence of fracture on the reservoir

Case 9 lacked a fault and the injected fluid flowed vertically, and the porosity change values were 0.16–0.38. In case 1, a fault existed in the formation, and the porosity change along the formation near the fault was 0.16–0.42. Case 1 had a wider diffusion range along the horizontal and vertical strata and had a larger porosity change range than case 9. The porosity change was the largest in the fracture where the porosity tended toward 0.5. Porosity and permeability were greater at the fault than in other areas. The higher values at the fault were critical in water transport so that the carbonate solution moved along the fault direction, increasing the reaction range of the fluid and the effect on the reservoir in this area, resulting in a larger change in porosity at the fault and its proximity (Fig 4).

(2) Influence of fracture width on the reservoir

The fault widths were 4 m in case 1, 8 m in case 3, and 10 m in case 4. Porosity change values were the largest (0.16–0.42) at a fault width of 4 m, with up to 80 m vertical migration along the fault. At a fault width of 8 m, the porosity change decreased to 0.16–0.38, with up to 60 m vertical migration. At a fault width of 10 m, the porosity change was the smallest (0.16–0.34), with up to 55 m vertical migration.
In the model of gradual fault widening, because of injecting a constant amount of fluid, a wider fault resulted in a larger flow area, fewer fluid–rock reactions, and a smaller area and amplitude of porosity change (Fig 5).

![Fig 5 Effect of fracture width on the reservoir (20 years)](image1)

(3) Influence of fluid injection velocity on the reservoir

The injection rates were 0.1 kg/s in case 7, 1 kg/s in case 1, and 2 kg/s in case 8. Porosity changes in the three cases were similar (0.16–0.4), but the reaction areas differed considerably. With an injection rate of 0.1 kg/s, the fluid reacted only within a few meters of the fracture. With an injection rate of 1 kg/s, the fluid reaction area was ~400 m horizontally and 80 m vertically. With an injection rate of 2 kg/s, the fluid reaction zone extended more than 500 m horizontally and 85 m vertically. As the injection rate increased, the reaction rate between the injected fluid and reservoir increased, the porosity changed more rapidly, and the degree and area of reservoir transformation increased (Fig 6).

![Fig 6 Influence of fluid injection velocity on the reservoir (20 years)](image2)

(4) Effect of fracture porosity and permeability on the reservoir

The fault porosity and permeability for cases 2, 1, 10, 11, and 12 were 0.2 and $1 \times 10^{-12}$, 0.3 and $1 \times 10^{-11}$, 0.4 and $1 \times 10^{-10}$, 0.2 and $1 \times 10^{-11}$, and 0.3 and $1 \times 10^{-10}$, respectively. Under low porosity and permeability, fluid migration within the reservoir and along the fault direction was weak after injection, but the amount of migration along the vertical fault direction increased after accumulation in the fault. However, fluid injection into a fracture with good porosity and permeability considerably enhanced migration along the fracture direction and transformation of the reservoir. Fluid injection from the bottom of the fault under greater porosity and permeability caused a rapid fluid migration, a larger influence range at the top of the fault, and stronger reservoir transformation (Fig 7).

![Fig 8 Effect of fracture porosity and permeability on the reservoir](image3)
The fault lengths were 40 m in case 6, 83 m in case 1, and 100 m in case 5. The corresponding reservoir response ranges were 350 m, 400 m, and 450 m, respectively. Longitudinally, change was not obvious, extending ~70 m. When the fault cut into the stratum over a short distance, the fluid accumulated near the fault, and the influence length along the transverse direction was short. When the fault cut into the formation at a greater distance, the fluid moves along the fault and reacts with the formation, increasing the response length along the transverse direction (Fig 8).

4.3. Trapping mechanism

CO₂ sequestration technology is one of the safest and most environmentally friendly technologies for effective CO₂ emission reduction. It is also critical to increase foreign exchange and even achieve carbon neutrality. CO₂ filling into a reservoir causes minerals and fluids in the reservoir to react and becomes locked within the formation in minerals, such as calcite and iron dolomite. Figure 9 shows the CO₂ fluid and mineral sequestration in different cases. The dissolution captures first increases, then decreases, whereas the mineral capture first decreases, then increases. The dissolved storage accounts for less than 1% of the total storage, and the mineral capture, the main type of storage, accounts for more than 99% of it.

Simultaneously, after the CO₂ fluid enters the reservoir, it migrates and spreads to the tail of the plume and generates many carbonate shells, such as calcite shells, blocking CO₂ diffusion. It has a positive significance for geological CO₂ storage. CO₂ fluid filling can transform the formation and function to seal the CO₂ in the formation, resulting in a mutual positive impact.
5. Conclusion

(1) Faults guide fluid migration within reservoirs, and fluids can migrate and react with the reservoir more readily in reservoirs containing faults.

(2) The fracture’s shape controls the fluid reaction and reservoir when fluid is injected. When a fracture is wide, fluid accumulates within it, the reaction within the reservoir is weaker than in the case of a narrow fracture, and the change in reservoir porosity is small. A long fracture causes a longer fluid migration distance and prevents fluid from accumulating. When the response range is small, the reservoir response intensity is weak, and porosity improvement is not very strong. A wide response range positively affects the porosity of large reservoirs.

(3) Fracture porosity and permeability conditions considerably influence fluid reaction and reservoir control. Under better porosity and permeability conditions, more fluid moves to the internal reservoir, reaction with the reservoir is stronger, and reservoir conditions are enhanced.

(4) The flow rate of the injected fluid is critical for reservoir control. When the injection flow rate is greater, more fluid accumulates within the reservoir in a unit of time, reaction with the reservoir is stronger, and the improvement of reservoir pore conditions is enhanced.

(5) After a certain amount of fluid has been injected, carbonate shells containing calcite are generated at the diffusion plume, hindering CO₂ diffusion and has a positive significance for the geological sequestration of CO₂.

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