

Original Paper

Molecular dynamics simulation for effect of stress on quartz dissolution: Implication on the development of high-quality reservoirs in foreland basins

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ABSTRACT

The dissolution of unstable minerals such as feldspar and carbonate is currently recognized as the primary cause of the dissolution pores in most clastic rock reservoirs globally. However, research has shown that quartz dissolution pores generally occupy a certain proportion in foreland basins typified by the Kuqa Depression. This paper studied the dissolution characteristics of quartz through the thin section analysis of the Cretaceous Bashijiqike Formation reservoir in the Kuqa Depression and molecular dynamics simulations, the findings profoundly clarify the influence of stress on quartz dissolution. It was found that the dissolution of quartz grains in the study area is quite common based on thin section observations. The molecular dynamics simulation experiments comprise two sets of experiments: umbrella sampling and molecular dynamics simulation of dissolution process. Through the umbrella sampling, it was found that under lateral compressive stress conditions, the free energy barrier for quartz dissolution is reduced. In molecular dynamics simulation experiments, there is a notable substance exchange process between quartz and the solution, ultimately forming a transition layer with a thickness of several angstroms, this layer exhibits greater thickness under lateral compressive stress conditions. In the simulated closed fluid mineral reaction system, the dissolution products of quartz enter the solution for a period of time, then ultimately reprecipitate on the surface of quartz. Through thin section analysis and molecular dynamics simulation research, the atomic level process of quartz dissolution under lateral compressive stress conditions has been elucidated, it may provide a new perspective on the formation mechanism of deep and ultra-deep high-quality clastic reservoirs.

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1. Introduction

Mineral dissolution is an important prerequisite for the formation and development of the deep and ultra-deep secondary pore type high-quality clastic reservoir (Dutton and Loucks, 2010; Feng et al., 2016; Nguyen et al., 2018). The dissolution of unstable minerals such as feldspar and carbonate is currently the main genetic type of reservoir space dominated by secondary pores in

the world (Yu et al., 2008; Cao et al., 2014). Quartz is a common stable mineral that is relatively difficult to dissolve (Futera et al., 2017). However, based on a review of existing literature and our research, we found that quartz dissolved pores can also occupy a certain proportion in reservoirs in foreland basins, and the content of quartz dissolved pores is relatively low or not reported in depression basins and graben basins (Table 1).

Quartz, as an important mineral component in reservoirs, has always been a focus of research on its impact on reservoirs. As a rigid particle, quartz can fracture under tectonic stress, generating secondary pores and fractures (Cui et al., 2024), and it also plays a critical role in enhancing reservoirs' resistance to compaction and preserving primary pores (Gao et al., 2019a; Ye et al., 2024).

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Table 1
Statistics on quartz dissolution in reservoirs of different types of basins.

Basin type	Country	Basin	Formation	Depth, m	Quartz content in reservoir, %	Description or percentage of quartz cement, %	Description or percentage of quartz grains dissolution, %	Ref.
Depression Basin	China	Junggar Basin	Baikouquan	2500–3700	7.3–30	Common	–	Yu et al. (2023)
	China	Ordos Basin	Shihezi	3497.4–4487.1	–	3.9	–	Gao et al. (2019b)
	China	Ordos Basin	Yanchang	–	55.34	Common	–	Zhang et al. (2022)
	Algeria	Illizi Basin	Unit IV-3	2763.4–2801	72.64	4.06–15.6	–	Benayad et al. (2019)
Graben Basin	America	Illinois Basin	Aux Vases	2851–2873.8	–	Minor	–	Montgomery and Leetaru (2000)
	Russia	East Siberia Craton	Nepa	3013–3340	60–80	Strong	–	Shaldybin et al., 2023
	Libya	Murzuq Basin	Hawaz	–	60–98	4–16	Grains pressure dissolution -	Abouessa and Morad (2009)
	Egypt	Shoushan Basin	Khatatba	3795	>95	Many	–	Shalaby et al. (2014)
Foreland Basin	Bengal	Bengal Basin	Bhuban	2691–2792	44–54	Abundant	–	Islam, 2009
	Yemen	Sabatayn Basin	Kuhlan	2698–2714	49.1–53.5	–	–	Al-hasani et al. (2018)
	China	Songliao Basin	Yingcheng	2263.7	–	–	0.08	Lu et al. (2018)
	China	Bohai Bay Basin	Shahejie	3431.3	41.9	–	0.15	Wang et al. (2013)
Foreland Basin	China	Bohai Bay Basin	Shihezi	>3500	89.7	Many	A small amount	Wang et al. (2023)
	America	Piceance Basin	Mesaverde	1296.2–1939	40–60	1–15	0.3*	Stroker et al. (2013)
	Austria	North Alpine	Puchkirchen	–	25–70	–	Grains partly dissolved	Gross et al. (2015)
	America	Appalachian	–	–	–	Common	–	Castle (1998)
Foreland Basin	South Africa	Main Karoo Basin	Ecca Group	1300–2300	18.4–31.8	Exis	Grains pressure dissolution	Baiyegunhi et al. (2017)
	China	Sichuan Basin	Xujiahe	3400–3700	–	–	Common	Jiang et al. (2009)
	China	Tarim Basin	Bashijiqike	2280–2340	18–59	Exist	0.01–1.65	This study
	China	–	–	4846–8080	–	–	–	–

Note: “–” in the table representatives the relevant content is not mentioned in the cited paper. The data with “*” is satisfied from thin sections in the cited paper.

Previous studies have shown that quartz mainly dissolves under alkaline conditions (Knauss and Wolery, 1988; Guo et al., 2013; Crundwell, 2017; Tian et al., 2022; Li et al., 2022), but in the presence of organic acids, the complexation between silica and organic acids, as well as the formation of complexes between the H⁺ ions and bridging oxygen atoms in Si-O-Si bonds, can also promote the dissolution of quartz (Yu et al., 2014; Wan et al., 2014). Additionally, temperature and pressure exert a significant influence on quartz dissolution. Physical simulation experiments have demonstrated that at a pressure of 23 MPa, temperature has a promoting effect on the dissolution of quartz within a specific range (20 °C to 374 °C); beyond 374 °C, the dissolution rate of quartz begins to decrease. In contrast, at a pressure of 33 MPa, the dissolution rate continues to increase even as temperature rises to 400 °C, before eventually declining. These results indicate that temperature and pressure can synergistically promote quartz dissolution under certain conditions (Zhang et al., 2015). Notably, different types of basins may undergo diverse diagenetic environments, characterized by variations in temperature, pressure, and fluid pH (Jiang et al., 2009; Wang et al., 2018, 2020; Li et al., 2022). Given this variability, diagenetic environment changes alone cannot explain the relatively higher proportion of quartz dissolution in foreland basins. Instead, the most distinct difference between foreland basins and the other two basin types during burial is their experience of intense lateral compressive stress. Can intense lateral compressive stress enhance quartz dissolution?

From the perspective of dissolution, the microscopic mechanism is the origin of macroscopic dissolution kinetics (Martin et al., 2021). Conventional microscopic characteristics of dissolution phenomena are generally investigated using various electron microscopes (e.g., polarizing microscopy, scanning electron microscopy), mainly primarily at the micrometer scale and above. In physical simulation experiments investigating quartz dissolution under varying temperature and pH conditions, honeycombed dissolution pores of quartz particles are observed (Chen et al., 2015). The key microscopic features of quartz dissolution identified via thin section analysis include: (1) the formation of serrated or harbor like edges resulting from dissolution; (2) particle dissolution residual; (3) pressure dissolution at grain contact (Qiu et al., 2002; Zhong et al., 2007).

Molecular dynamics simulation can extend the scale of research to the molecular and atomic levels, which is of great significance for revealing the dissolution process and mechanism of minerals from the micro-nano perspective under lateral compressive stress in foreland basins. The research on molecular dynamics simulation mainly involves using methods at different theoretical levels to characterize the molecular level details of dissolution reactions, including classical molecular dynamics simulation (CMD) (Rimsza et al., 2018), kinetic Monte Carlo (KMC) simulation (Nangia and Garrison, 2009; Kurganskaya and Lutttge, 2013), and quantum mechanical calculations (AIMD, DFT) (Xiao and Lasaga, 1996; Dellostritto et al., 2014; Zhang and Liu, 2014). Monte Carlo simulations indicate that the gradual dissolution mechanism is more similar to the steady-state dissolution process of quartz water systems (Nangia and Garrison, 2009). Ab initio calculation indicates that the presence of Na⁺ under alkaline conditions accelerates the hydrolysis reaction of Si-O bonds in quartz, while Ca²⁺ and Mg²⁺ are the opposite (Zhang and Liu, 2014). However, these two methods have two key limitations: they require extensive computational resources, and on the other hand, they cannot adequately explain the dynamic process of chemical bond breaking and formation during mineral dissolution. In classical molecular dynamics (CMD), NaOH molecules are introduced into the reaction system to create an alkaline solution environment. Simulation demonstrate that Na⁺ ions adsorb on the

Based on the previous molecular dynamics simulation research, combined with the anatomy of the geological data of the Kuqa Depression, in this study, we take the Kuqa foreland basin in the Tarim Basin in western China as the research background (Fig. 1). On the one hand, we conduct microscopic thin section observation and research on the dissolution characteristics of quartz in the Cretaceous Bashijiqi Formation clastic reservoir in the Kelasu structural belt of the Kuqa Depression (Fig. 1(b)). On the other hand, a series of molecular dynamics simulation

experiments were conducted on the dissolution of quartz under formation temperature, pressure, and lateral compressive stress conditions. In order to revealing the reason for the relatively high dissolution percentage of quartz in the foreland basins, thereby offering a new perspective for the formation of high-quality deep and ultra-deep reservoirs.

2. Geological setting

Kuqa Depression is a Mesozoic–Cenozoic continental foreland basin superimposed on the Paleozoic marine craton basin in the Tarim Basin. It is tectonically located in the northern Tarim Basin and southern part of the South Tianshan orogenic belt (Yang et al., 2020) (Fig. 1(a)). Previous studies have shown that the Lower

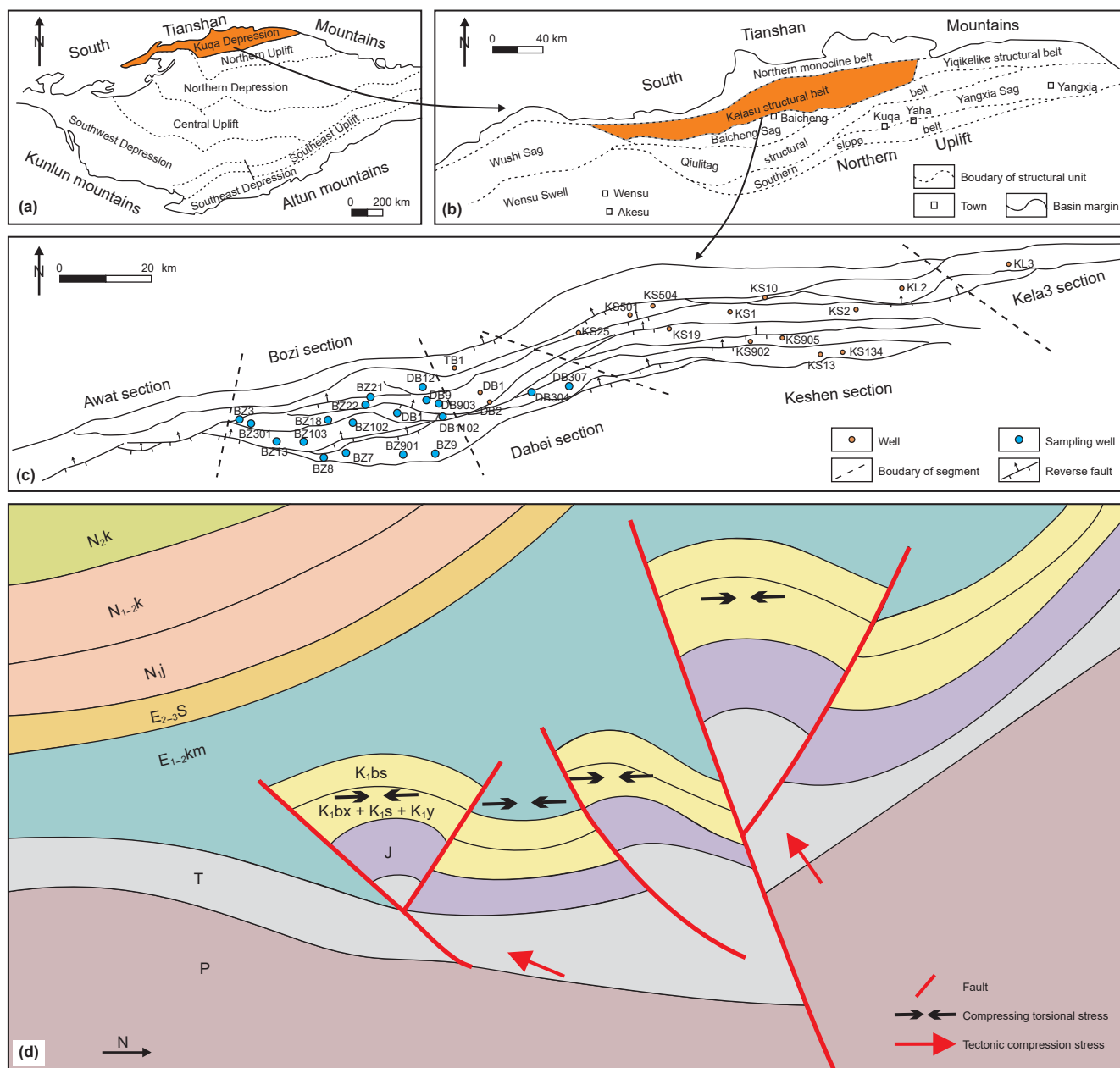


Fig. 1. Geologic background. **(a)** Structural map of Tarim Basin (modified after Liu et al., 2018). **(b)** Structural map of Kuqa Depression (modified from Liu et al., 2018). **(c)** Geological profile map of the Kelasu structural belt (modified from Liu et al., 2022). **(d)** Pattern diagram of the layered model of the faulted anticline reservoir in the Kelasu structural belt (modified from Li et al., 2017b).

Cretaceous reservoirs in the Kelasu area have undergone four stages of development and evolution: early-stage shallow burial, middle-stage slow deep burial, late-stage rapid deep burial, and final-stage abrupt deep burial. During the gradual deep burial process, the reservoirs experienced intense lateral compressive stress. The maximum horizontal paleo-effective stress at each stage in this region, measured via the acoustic emission method, was approximately 35, 60, 75 MPa, and over 80 MPa, respectively (Wang et al., 2022). The Late Cretaceous Yanshan Movement caused the overall uplift of the Kuqa Depression, leading to the absence of the Upper Cretaceous strata (Wang et al., 2022). In the early and long-term alkaline environment, there was poorly developed siliceous cementation. As the burial depth gradually increased, temperature rose, and the tectonic compression occurred, the pressure solution between grains provided the primary source of siliceous material (Mao, 2019). From bottom to top, the Lower Cretaceous strata consist of the Yageliemu Formation (K_{1y}), Shushanhe Formation (K_{1s}), Baxigai Formation (K_{1bx}), and Bashijiqike Formation (K_{1bs}) (Zhang et al., 2021) (Fig. 2(a)). The rock types of the Bashijiqike Formation reservoir are dominated by medium to fine grained feldspar lithic sandstone and lithic feldspar sandstone. During this sedimentary period, thick sandbodies were widely developed in the delta front (Zeng et al., 2020).

3. Samples, method and experimental design

3.1. Selection and processing of geological samples

Geological samples were taken from 19 core wells of Cretaceous Bashijiqike Formation in the Kuqa Depression (Fig. 1(c),

Table S1). These samples are mainly composed of feldspar lithic sandstone and lithic feldspar sandstone, with porosity ranging from 2% to 10% and an average of 5.42%. Typical core samples are shown in Fig. 2. Prior to thin-section preparation, samples were impregnated with blue epoxy resin to enhance the visibility of pore characteristics. Subsequently, the samples were subjected to rough grinding, medium grinding, fine grinding and final polishing to obtain the thin slice samples used in this study. The Zeiss optical microscope was used to observe and analyze the dissolution characteristics of quartz particles in thin section samples. Quantitative statistical analysis was conducted on the total porosity, total dissolution porosity, as well as porosity generated by dissolution of quartz particles, quantified via the area method (i.e., the proportion of the target area).

3.2. Molecular dynamics simulation experiment design

The quartz crystal structure file used in this study was obtained from the crystal structure database of the materials studio (MS) software. A series of preprocessing steps were performed as follows: the initial quartz crystal was cut along the (010) crystal plane, followed by expansion 3 times and 4 times along the a and b directions, respectively (the final obtained crystal parameters were: $a = 25.51 \text{ \AA}$, $b = 24.55 \text{ \AA}$, $c = 25.33 \text{ \AA}$, $\alpha = \beta = \gamma = 90^\circ$). Subsequently, unsaturated silicon atoms formed after crystal surface cutting were compensated with two hydroxyl groups (a process referred to as surface hydroxylation), yielding a quartz crystal model. Both the upper and lower surfaces were composed of Q² groups (Fig. 3(a)) (the n in Q ^{n} notation represents the number of bridging bonds connecting the Si to the neighboring Si site of

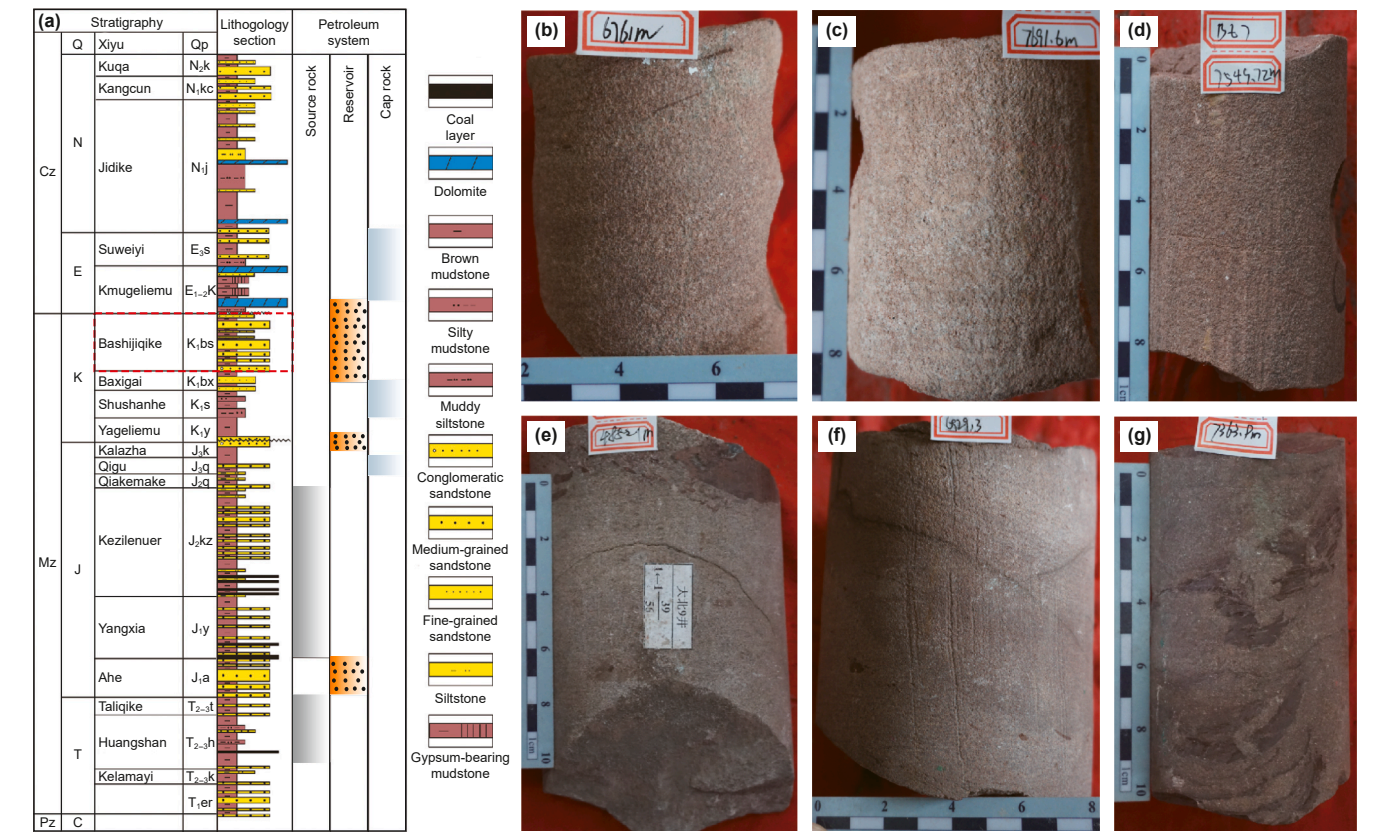


Fig. 2. Stratigraphic diagram of Kuqa Depression (Fig. 2(a)) (modified from lai et al., 2017), the red dashed box indicates the studied formation. C = Carboniferous; Cz = Cenozoic; E = Eocene; J = Jurassic; K = Cretaceous; Mz = Mesozoic; N = Neogene; Pz = Paleozoic; Q = Quaternary; T = Triassic. Typical sampling core of Bashijiqike Formation in Kelasu structural belt (Fig. 2(b)–(g)). (b) BZ102–6761 m, sandstone; (c) BZ9–7691.6 m, sandstone; (d) BZ7–7549.72 m, sandstone; (e) DB9–4852.1 m, sandstone; (f) DB304–6929.3 m, sandstone; (g) DB307–7363.9 m, gravel-bearing sandstone.

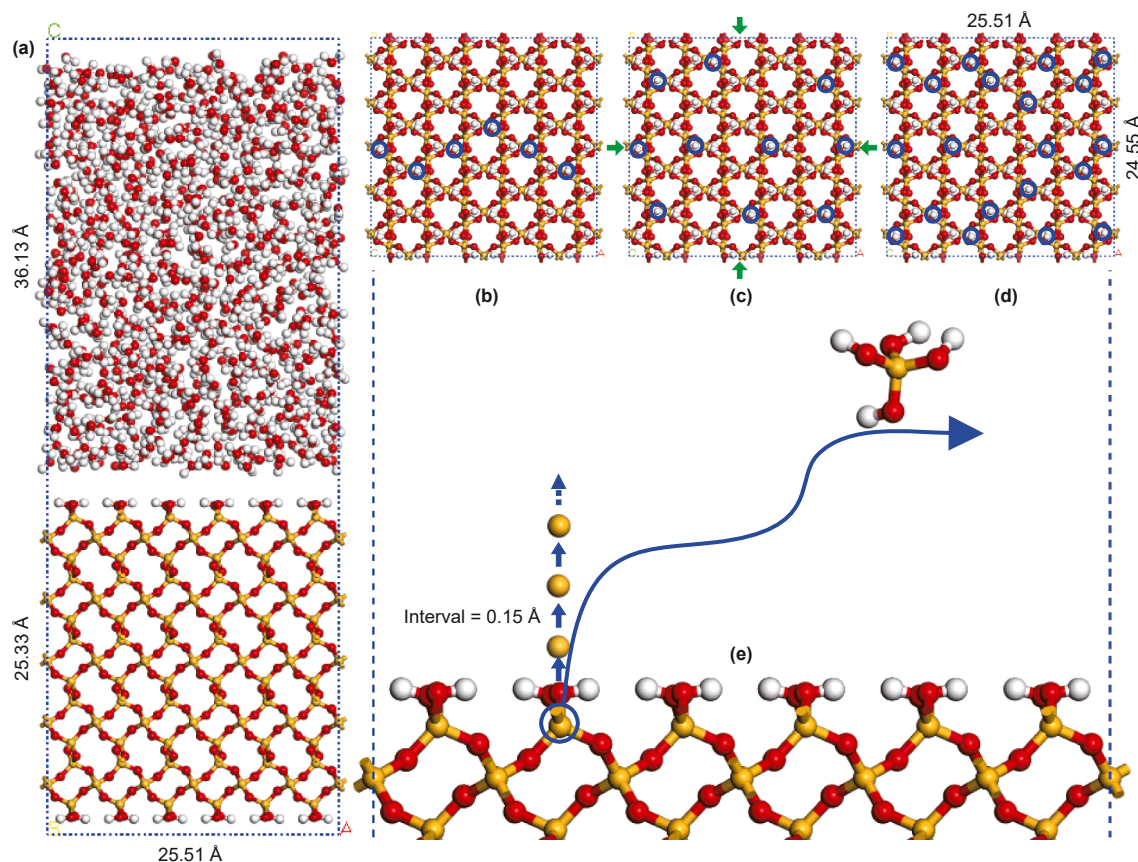


Fig. 3. Schematic diagram of the reaction model, model dissolution, and umbrella sampling. (a) Basic reaction model. (b) The top view of the quartz crystal model shows the surface of the model with pH = 7.5. Blue circles in the figures represent deprotonation positions on the quartz crystal surface. (c) The top view of the quartz crystal model shows the surface of the model with pH = 9.5. The green arrow indicates the direction of strain applied to the model. (d) The top view of the quartz crystal model shows the surface of the model with pH = 11. (e) Schematic diagram of the umbrella sampling process. For clarity, water molecules and sodium ions have been omitted. Yellow spheres represent silicon atoms, red spheres represent oxygen atoms, and white spheres represent hydrogen atoms.

quartz, and the number of hydroxyls connecting to the Si is $4-n$ (Nangia and Garrison, 2009). A water box matching the model specifications was established using the “Amorphous Cell” module of the MS software, and the quartz crystal model and water box were combined to form the basic model used in this study using the MS “Build Layer” module (Fig. 3(a)).

In developmental process of the Cretaceous Bashijiqike Formation reservoir in the study area, fluid properties undergo a complex evolution from alkaline to weakly acidic, then to alkaline and finally to acidic conditions (Li et al., 2017a). Furthermore, given the background of intense lateral compressive stress in foreland basins, we investigated the effects of solution pH and lateral compressive stress on the quartz dissolution process (encompassing two lateral compressive stress environments and four pH conditions). These two sets of experimental conditions were achieved by making slight adjustments to the basic model. For quartz, a strong linear relationship exists between stress and strain when the strain is 0.02 or lower (Chowdhury et al., 2016). In the simulation, since direct stress application to the model is not feasible under the simulation conditions, strain was applied along the length and width directions of model to mimic lateral compressive stress conditions in geological conditions (with the strain in the length and width directions of the model is set to 0.02).

Changes in solution pH can alter the protonation state of surface hydroxyl groups, influence mineral surface charge, thereby control some key processes (Lyu et al., 2019), such as mineral dissolution mechanism and reaction rates (Nangia and Garrison,

2008). There exists a special pH value known as the zero charge point (PZC), at which the hydroxyl groups on mineral surface are in a neutral state with zero net charge, and the PZC of quartz is 2 (Fuerstenau, 2005). Different pH conditions were simulated by adjusting the degree of protonation of hydroxyl groups on quartz surface to achieve varying surface charge densities. Surface charge densities of -0.03 , -0.06 , and $-0.12 \text{ C}\cdot\text{m}^{-2}$ correspond to pH values of 7.5, 9.5, and 11, respectively (Krouitil et al., 2015) (Fig. 3(b)–(d)). Accordingly, we selected four pH conditions (2, 7.5, 9.5, and 11) for this study. All deprotonated reaction systems maintained the electrical neutrality of the model system by adding Na^+ to the solution. The configurations of the four reaction systems (i.e., pH 2, 7.5, 9.5, 11) are presented in Table 2.

This study conducted two sets of molecular dynamics (MD) simulations. This first was an umbrella sampling MD simulation to quantify the difficulty of quartz dissolution (i.e., to obtain the free energy of the dissolution reaction), referred to as Experiment 1. This experiment focused on the four aforementioned pH conditions and two lateral compressive stress environments, and involved two main procedures: equilibrium molecular dynamics simulation (under isothermal isobaric ensemble, NPT) and umbrella sampling molecular dynamics simulation (under canonical ensemble, NVT), with a time step of 0.25 fs. Many features related to surface dissolution typically only appear during precise molecular dynamics simulations over extended periods (Manzano et al., 2015), thus a kinetic calculation of 250 ps was performed for each stage of the Experiment 1. The temperature and pressure

Table 2
Model configuration under different pH conditions.

Solution pH value	Quartz model	Water box	
	surface charge density/C·m ⁻²	H ₂ O number	Na ⁺ number
2	0	750	0
7.5	−0.03	750	3
9.5	−0.06	750	5
11	−0.12	750	10

conditions for Experiment 1 were 364 K and 30 MPa (corresponding to the approximate temperature and pressure conditions of the 3000 m formation in the Kuqa Depression). Under this deep geological temperature and pressure environment, equilibrium molecular dynamics simulations were performed on the experimental models (for the four aforementioned pH values) under two scenarios: with lateral compressive stress (hereafter referred to as the “stressed conditions” for brevity) and without lateral compressive stress (hereafter referred to as the “stress free conditions” for brevity). The equilibrium configuration obtained from the equilibrium molecular dynamics simulation stage was then subjected to conduct the umbrella sampling. The sampling interval was set to 0.15 Å (Fig. 3(e)), and the target silicon atom (i.e., the umbrella sampling object) was constrained at each sampling position using a harmonic bias potential: $U = (k/2) \cdot (x - x_i)^2$, where x_i is the reference distance of the i -th sampling position (Henning-Knechtel et al., 2022) and the elastic coefficient (k) was set to 500. For each pH value, 35 umbrella sampling experiments were conducted under stressed and stress free conditions, respectively (totally 280 umbrella sampling experiments). These experiments involved gradually pulling a single silicon atom from the quartz surface to a position approximately 5 Å above the surface. The position information of the target silicon atom in each trajectory file was recorded, and the free energy profiles under different conditions were subsequently derived using weighted histogram analysis method (WHAM) (Kumar et al., 1992; Roux, 1995).

Another set of experiments was the molecular dynamics simulation investigating quartz dissolution characteristics under the background of deep formation temperature, pressure and lateral compressive stress (recorded as Experiment 2). In Experiment 2, a 3.5 ns dynamic simulation with temperature and pressure conditions of 442.15 K, 59 MPa and alkaline environment (pH = 11) was conducted under stressed and stress free conditions (approximately the temperature and pressure conditions of the 6000 m formation in the Kuqa Depression), the molecular dynamics calculations were performed under the NVT ensemble, with a time step of 0.5 fs. Simulation results were visualized using visual molecular dynamics (VMD) software (Humphrey et al., 1996).

All molecular dynamics simulations conducted in this study were implemented using the open-source LAMMPS code. LAMMPS supports simulations of materials from atomic to mesoscopic to continuum scales, and is widely used in fields such as materials science, chemical physics, and biomolecules (Plimpton, 1995; Thompson et al., 2022). The temperature and pressure were modulated using the Nosé–Hoover thermostat (Nosé, 1984; Hoover, 1985). Both experiments were performed using the ReaxFF reactive force field, which can describe the processes of bond breaking and formation in chemical reactions (Guo et al., 2024), and the structural characteristics of quartz (Fig. S1). During the development of this force field, researchers incorporated quantum mechanics (QM) calculations into the force field parameter training set. Simulation based on this force field can ensure the accuracy of chemical reactions while enabling the study of chemical reaction systems over relatively large time

scales. The ReaxFF reactive force field is a bond-order-dependent potential, and its total interaction energy can be written in the following form (Hahn et al., 2018):

$$E_{\text{sys}} = E_{\text{bond}} + E_{\text{val}} + E_{\text{tor}} + E_{\text{over}} + E_{\text{under}} + E_{\text{lp}} + E_{\text{vdWaals}} + E_{\text{coulomb}} \quad (1)$$

In Eq. (1), E_{bond} is bond energy, E_{val} is valence angle energy, E_{tor} is torsion angle energy, E_{over} is over-coordination penalty energy, E_{under} is under-coordination penalty energy, E_{lp} is lone-pair energy, and the nonbonded interactions terms include the van der Waals energy (E_{vdWaals}) and the coulomb energy (E_{coulomb}).

4. Results

4.1. Dissolution characteristics of quartz particles

The contact relationships between mineral grains observed in thin sections mainly include line contact, concave-convex contact, as well as point contact, and the degree of dissolution of quartz particles is relatively high. The types include edge dissolution of quartz particles (Fig. 4(a)–(c)) and internal dissolution (Fig. 4(d)–(f)). The dissolution area of a single quartz particle can even reach more than 50% of the entire particle area (Fig. 4(f)). In areas with strong tectonic stress, particles are mainly in linear contact, with a small amount of concave-convex contact and point contact. Overall, the contact boundary is relatively flat, and dissolution mainly occurs along the contact surface (Fig. 4(a)–(d), (f)), mainly manifested as serrated dissolution, with intermittent harbor like dissolution visible. Quartz overgrowth can be observed in the pores between particles (Fig. 4(d)). In areas with relatively mild stress, point contact is more common. Due to the more significant stress concentration effect, the pressure dissolution phenomenon is more pronounced at the point contact site, and the degree of development of harbor like dissolution is higher (Fig. 4(e)).

By carefully outlining the pore characteristics of different genetic types under thin section, the porosity of the thin sections derived from quartz particles dissolution was statistically analyzed (Fig. 5). The proportion of quartz particle dissolution pores in the secondary dissolution porosity and total porosity was relatively high, reaching over 50% or even higher (Fig. 5(d) and (e)). Acoustic emission paleostress test results from the study area (Zhang et al., 2014) show that as the maximum paleotectonic stress increases, the porosity of thin sections resulting from quartz particles dissolution also increases, and a strong positive correlation exists between these two factors (Fig. 6).

4.2. Molecular dynamics simulation based on deep formation environment of Kuqa foreland basin

4.2.1. Experiment 1: equilibrium molecular dynamics simulation stage

Statistically analyzed the radial distribution function between oxygen atoms on the surface hydroxyl (including surface hydroxyl oxygen and deprotonated hydroxyl oxygen) and the hydrogen atoms in water molecules during the equilibrium molecular dynamics simulation stage (Fig. 7), indicating that under higher pH conditions, the hydration degree of hydroxyl groups was higher.

4.2.2. Experiment 1: umbrella sampling stage

The potential of mean force (i.e., free energy) profiles of silicon atom dissolving from the quartz surface into the solution was obtained (Fig. 8). In acidic and weakly alkaline solution environments, the free energy barrier is higher than that in strongly

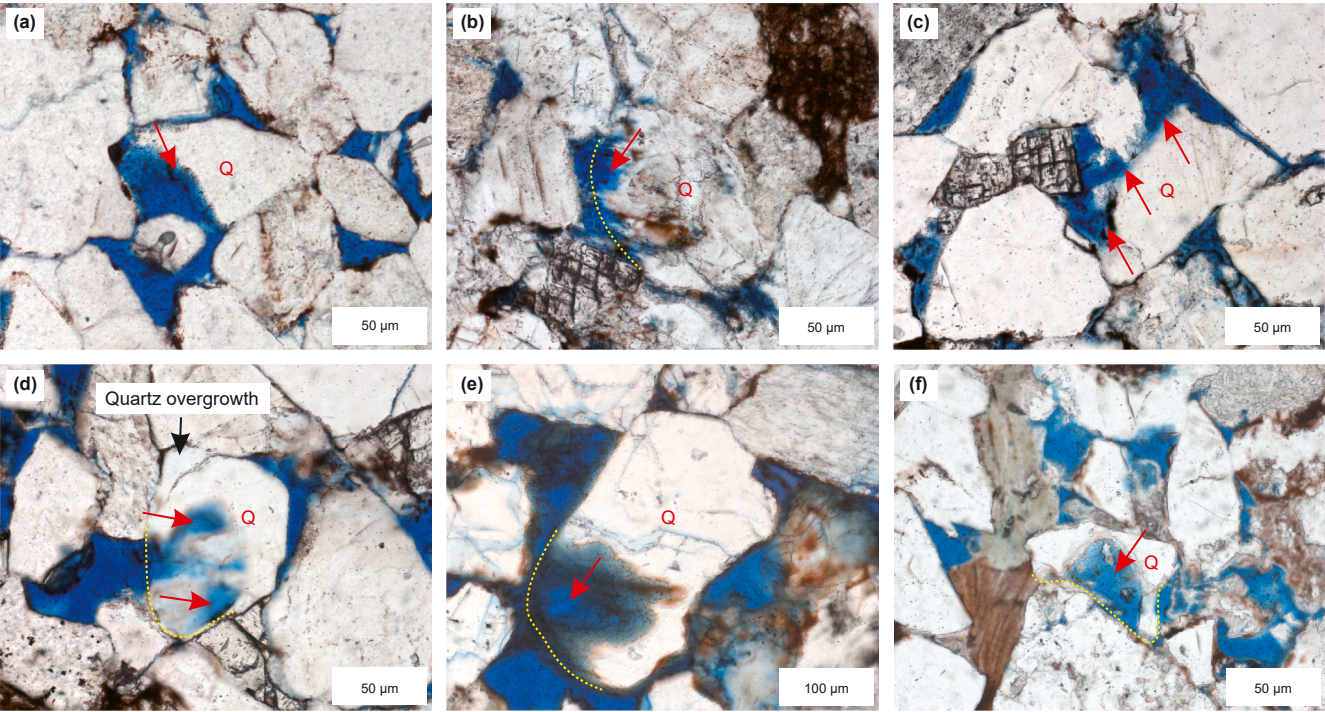


Fig. 4. Thin sections of Bashijiqi Formation of Kelasu structural belt. (a) BZ7-7744.26 m, the edges of quartz are dissolved into arc-shaped shapes; (b) BZ102-6761 m, edge dissolution of quartz particle; (c) BZ102-6763 m, multiple dissolution points at the edge of quartz; (d) BZ7-7745.16 m, multiple dissolution points inside the quartz particle; (e) BZ9-7679.7 m, internal dissolution of quartz particle; (f) DB12-5448.9 m, internal dissolution of quartz particle. The red letter Q in the picture refers to quartz grains, the red arrow indicates the location where quartz grains are dissolved, and the yellow dashed line represents the contour line of the dissolved quartz grains.

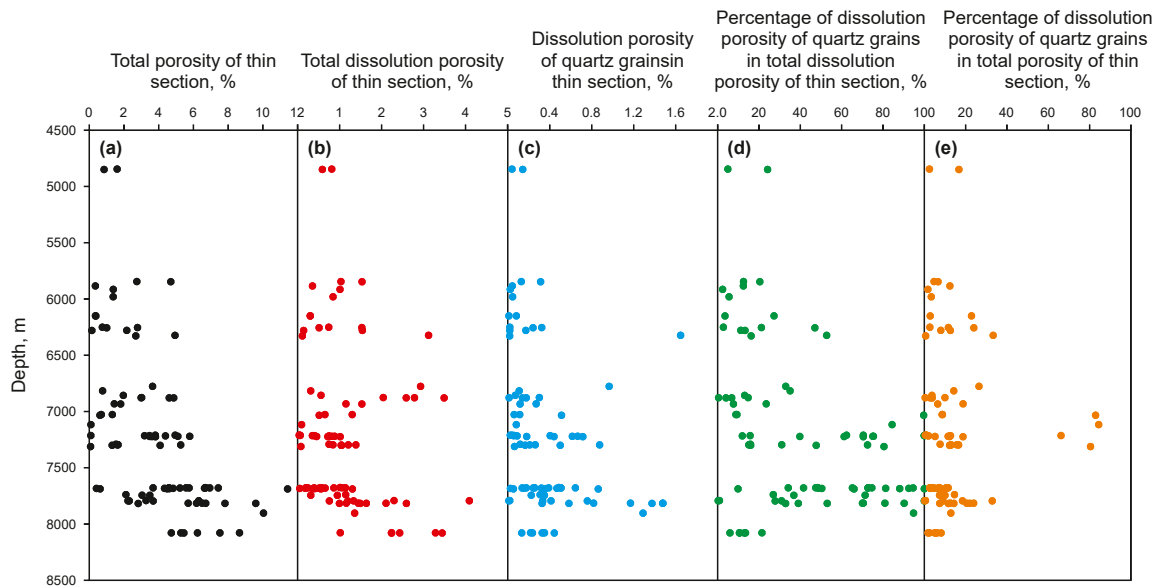


Fig. 5. Statistical characteristics of thin section porosity in the Bashijiqi Formation of Kelasu structural belt. (a) Total porosity of thin section; (b) total dissolution porosity of thin section; (c) dissolution porosity of quartz grains in thin section; (d) percentage of dissolution porosity of quartz grains in total dissolution porosity of thin section; (e) percentage of dissolution porosity of quartz grains in total porosity of thin section.

alkaline solution environments. After the application of lateral compression stress, the free energy barrier only slightly decreased in weakly alkaline environments ($\text{pH} = 7.5$); in contrast, the free energy barrier decreased significantly in strongly alkaline and acidic environments. For the four pH conditions selected in the experiment, the free energy barrier for the dissolution of a single silicon atom under stressed conditions (Fig. 8(b)) was lower than that under stress free conditions (Fig. 8(a)).

4.2.3. Experiment 2: quartz dissolution molecular dynamics simulation

Through molecular dynamics simulations under formation temperature, pressure, and alkaline conditions, quartz exhibits significant reaction characteristics. Material exchange occurred between quartz and solution (Fig. 9), mainly manifested as hydrogen and oxygen atoms of some water molecules in the solution approaching the quartz surface, as well as hydrogen and

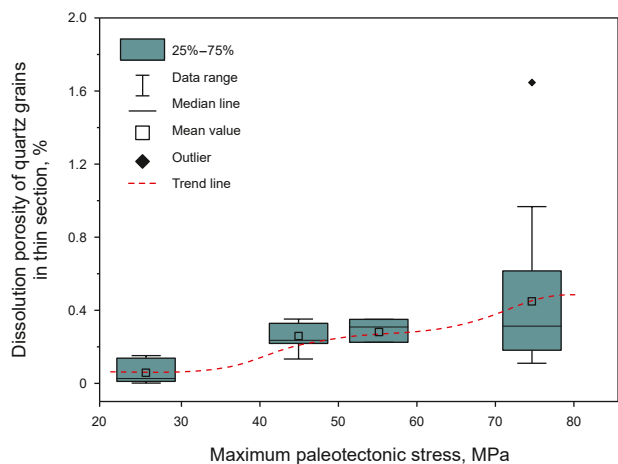


Fig. 6. The relationship between maximum paleotectonic stress and the dissolution porosity of quartz grains in thin section in Bashijiqike Formation.

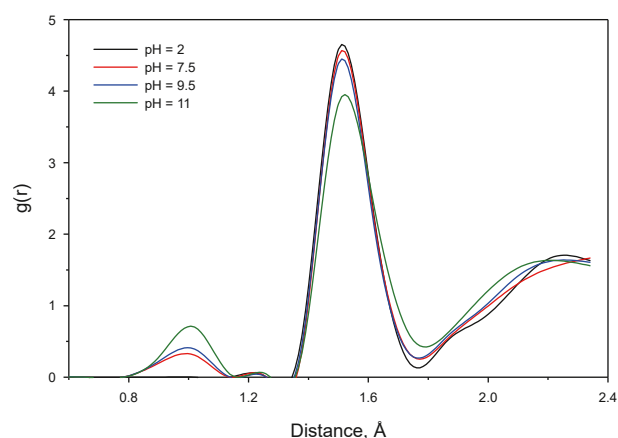


Fig. 7. Radial distribution functions for the oxygen atoms on the surface hydroxyl and the hydrogen atoms in water molecules.

oxygen atoms in hydroxyl groups on the quartz surface entering the solution. As the reaction progressed, hydrogen in water molecules slowly entered the interior of quartz through the quartz–water reaction interface, and the quartz surface structure

gradually transformed from a regular crystalline morphology to a slightly disordered atomic arrangement, this structure is referred to as the transition layer (Region II in Fig. 10). It is worth noting that under stressed conditions, in addition to the aforementioned atomic exchange, both oxygen atoms in water molecules and hydrogen atoms in hydroxyl groups on quartz surface diffuse into the transition layer (Fig. 9(e)–(h)), but this phenomenon was not observed under stress free conditions (Fig. 9(a)–(d)). Furthermore, the thickness of the transition layer is greater under stressed conditions (Fig. 9). The hydrogen atoms entering the transition layer bond with the internal bridging oxygen atoms, causing the Si–O–Si connection to break and form hydroxyl groups. Various forms of quartz species were observed within the transition layer (Fig. 10). The quantities distribution characteristics of hydrogen atoms and silicon atoms after the reaction were statistically analyzed (Fig. 11). Under stressed conditions, the amount of silicon atoms in the transition layer was higher than that under stress free conditions, and silicon atoms was present in the solution.

The dissolution-precipitation process at surface Q^2 sites was observed in the simulation, with a gradual dissolution process of Q^2 – Q^1 – Q^0 (Fig. 9(a)–(c), (e)–(g)) and a reprecipitation process of Q^0 – Q^1 (Fig. 9(c)–(d), (g)–(h)). The dissolution product of quartz is dominated by orthosilicate (H_4SiO_4) in Q^0 configuration (as shown in Fig. 9(c) and (g)). The core structural feature of this configuration is that a single silicon atom is covalently connected to four hydroxyl groups (–OH). This structure directly indicates that the Si–O–Si bond of the silicon atom has been completely broken, and the dissolution process of the single silicon atom has reached a completed state. In situ nuclear magnetic resonance (NMR) experiments provide direct evidence that orthosilicic acid (H_4SiO_4) is unstable under alkaline conditions: its hydroxyl group is prone to deprotonation reaction, converting to $H_3SiO_4^-$, which is thermodynamically spontaneous (Sefcik and Goddard, 2001). Additionally, density functional theory (DFT) studies have shown that the attack of O-terminal of negatively charged silicates on silicon atoms of neutral monomers (possibly Si–OH on quartz surfaces or other silicate monomers in solution) is a key step in forming Si–O–Si bonds (Xia et al., 2021). For the present study, $H_3SiO_4^-$ undergoes a condensation reaction with Si–OH groups on quartz surfaces (neutral monomers) to form Si–O–Si bonds, with the configuration transforming into Q^1 (Fig. 9(d) and (h)), this observation indicates the progression of the reprecipitation process on the quartz surface.

Use the potential energy and kinetic energy of the initial state system as a benchmark, the dynamic changes in potential energy

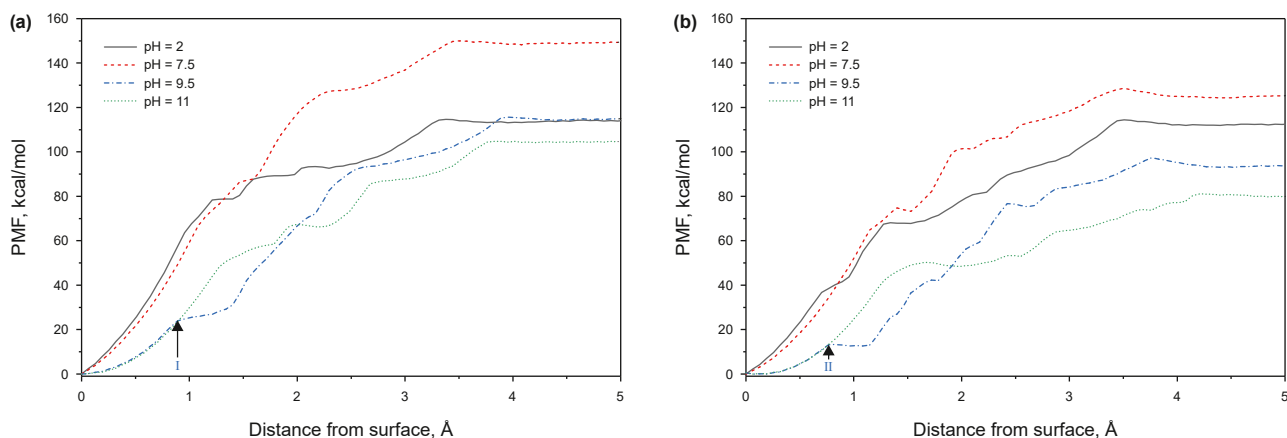


Fig. 8. The average force potential (PMF) (i.e. the free energy profile) of silicon atom dissolution obtained through umbrella sampling under four different solution pH conditions. (a) Simulation results under stress free conditions, (b) simulation results under stressed conditions. The roman numerals in the figures indicate the first inflection point of the free energy curve of alkaline solution environment (pH = 9.5), which will be analyzed in the discussion section (Fig. 13).

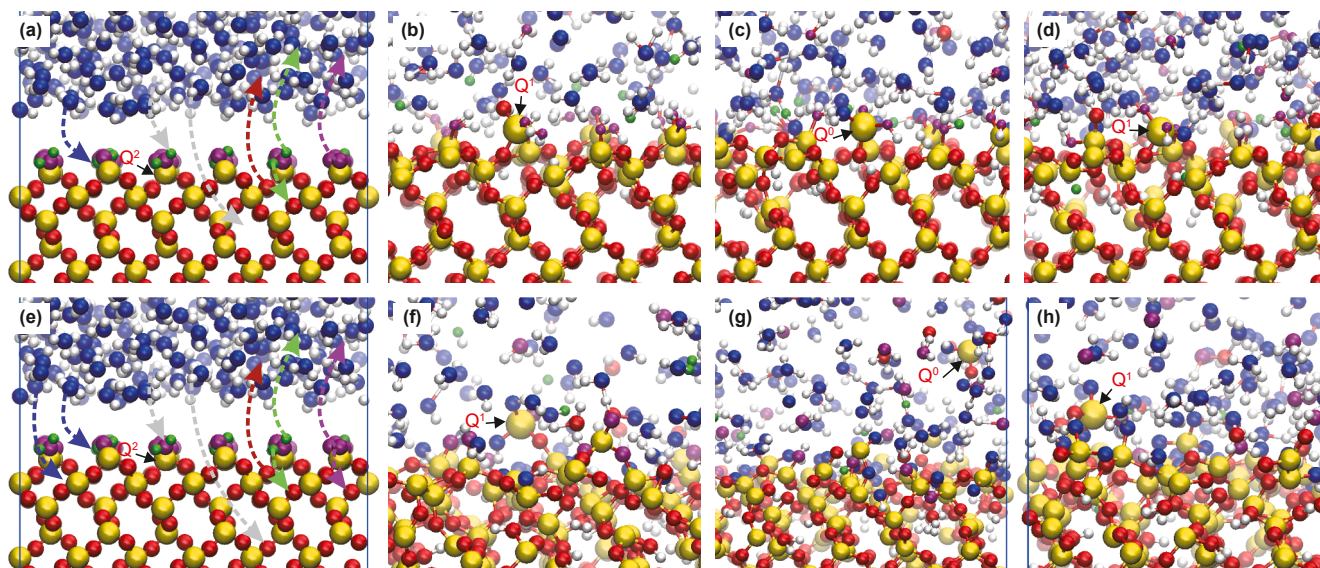


Fig. 9. Molecular dynamics simulation results of quartz reaction in the deep formation of 6000 m and alkaline solution environment (pH = 11). (a)–(d) show the experimental results under stress free conditions, and (e)–(h) show the experimental results under stressed conditions. (a) and (e) show the initial states under their respective conditions. The dashed lines indicate the direction of movement of the corresponding atoms in the subsequent reaction process, the light gray dashed lines indicate the direction of movement of water molecule hydrogen, the light blue dashed lines indicate the direction of movement of water molecule oxygen, the green dashed lines indicate the direction of movement of hydroxyl hydrogen on the surface of quartz, the purple dashed lines indicate the direction of movement of hydroxyl oxygen on the surface of quartz, and the red dashed lines indicate the direction of movement of bridge oxygen (–Si–O–Si–) inside quartz. The white ball in the picture represents water molecule hydrogen, the blue ball represents water molecule oxygen, the green ball represents surface hydroxyl hydrogen of quartz surface, the purple ball represents surface hydroxyl oxygen of quartz surface, the red ball represents internal bridging oxygen of quartz, and the yellow ball represents silicon atoms.

and kinetic energy of quartz during dissolution and reprecipitation were analyzed (Fig. 12). During the quartz dissolution process, both the potential energy and kinetic energy of the reaction system under stressed conditions are higher than those under stress free conditions. During the reprecipitation process, the potential energy of the reaction system under stressed conditions is slightly lower than that under stress free conditions.

5. Discussions

5.1. Differences in free energy curves (PMF)

By analyzing the configuration of the target silicon atom during the umbrella sampling process, we identified the reasons underlying the differences in free energy curves under stress conditions. The initial Q^2 group forming Q^1 group at the inflection point under both stress free and stressed conditions (Figs. 8 and 13). Under stress free conditions, when one of the Si–O bonds of initial Q^2 group breaks, hydrogen and oxygen from two water molecules in the solution combine with the breaking position to form Q^1 group (Fig. 13(a)–(c)). Under stressed conditions, when one of the Si–O bonds in the Q^2 group breaks, the breaking site is formed by the combination of hydrogen and oxygen from water molecules and hydrogen in the hydroxyl groups on the quartz surface (Fig. 13(d)–(f)). By comparing Fig. 13(a) and (d), the hydrogen required to form Q^1 group in the reaction is far from the reaction surface under stress free conditions, one of the reasons for the lower free energy of the Q^1 group under stressed conditions is that the material sources that form it are closer compared to those under stress free conditions.

5.2. Free energy barrier of the key processes

For the Q^2 quartz surface used in this simulation experiment, the results indicate that its dissolution involves two fundamental reaction processes: $Q^2 \rightarrow Q^1$ and $Q^1 \rightarrow Q^0$ (Fig. 9). Gibbs free energy,

as an important thermodynamic function, can determine the direction of chemical processes and control the driving force of dissolution reactions (Martin et al., 2019).

To compare and investigate the difficulty of Q^2 site dissolution on quartz surfaces under acidic and alkaline solution conditions, as well as the influence of lateral compression stress factors, the free energy changes of the two key processes $Q^2 \rightarrow Q^1$ and $Q^1 \rightarrow Q^0$ under four sets of simulated experimental environments were statistically analyzed (ΔG) (Fig. 14). The results showed that under the four solution conditions in the experiments, except for the stressed conditions with pH = 9.5, the free energy barrier of the $Q^2 \rightarrow Q^1$ process was significantly higher than that of the $Q^1 \rightarrow Q^0$ process (Fig. 14). This indicates that the occurrence of Q^2 site dissolution requires first overcoming the first Si–O bond connected to the quartz surface, this step demands higher energy and is the rate-limiting step of the entire dissolution reaction. Previous studies have also shown that the most difficult part of dissolving atomic planes is the removal of the initial few molecular units (Berner and Morse, 1974). It further indicates that the quartz dissolution is a gradual process, this gradual dissolution mechanism of Q^n ($n = 2$ or 3) sites on a quartz surface is closer to the steady-state dissolution process of the quartz–water system compared to the one-step direct dissolution mechanism (Nangia and Garrison, 2009).

However, when stress factors intervene in the reaction process, as the pH value of the solution gradually increases to the alkaline region (i.e., pH = 9.5), the free energy required for the $Q^1 \rightarrow Q^0$ process exceeds that of the $Q^2 \rightarrow Q^1$ process, this step becomes a limiting step in the dissolution reaction (Fig. 14). Moreover, from the results of the four sets of simulation experiments, the addition of stress conditions can significantly reduce the free energy barrier at each stage of the Q^2 site dissolution, which reflects the significant promotional effect of stress on quartz dissolution. On the other hand, the addition of stress conditions in some strongly alkaline environments (pH = 9.5) changes the reaction limiting steps of dissolution reaction, which may exert a more profound impact on the reaction mechanism.

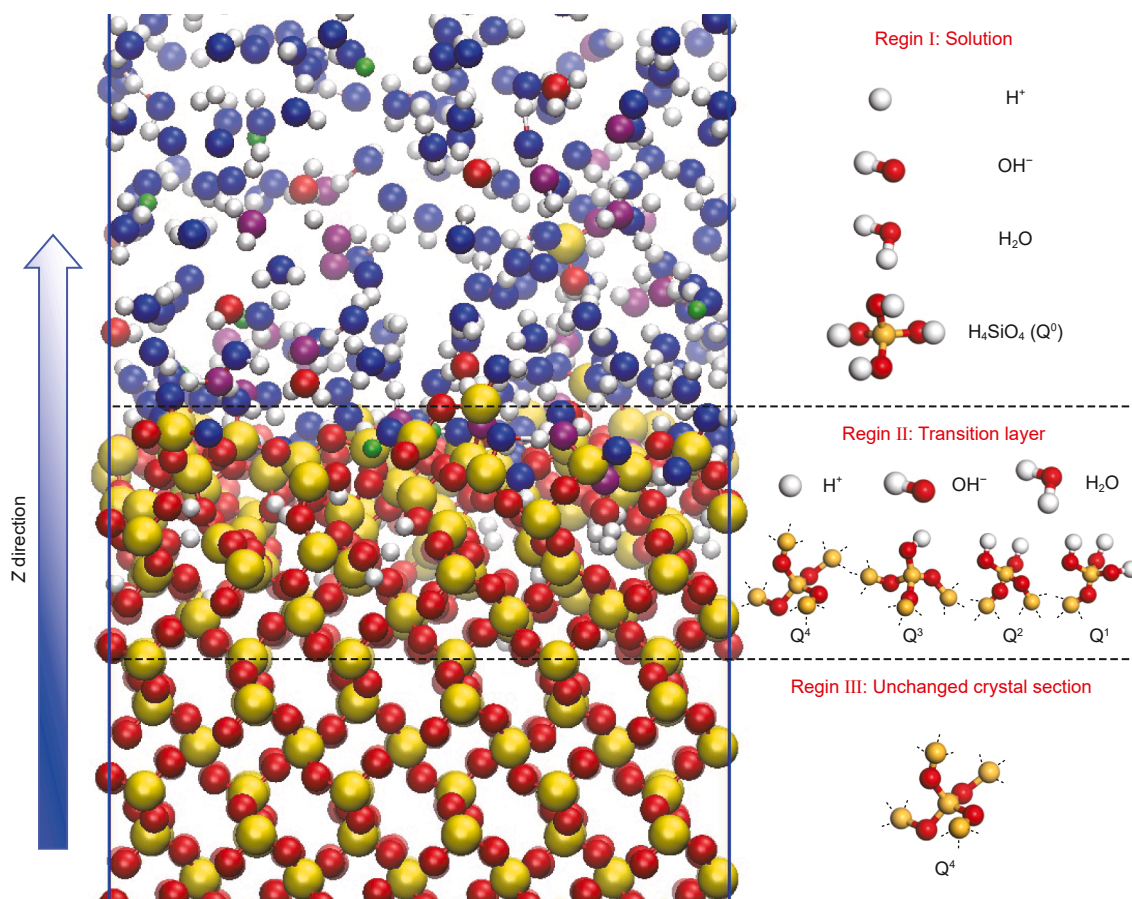


Fig. 10. Quartz dissolution characteristic under stressed conditions of deep formation of 6000 m (442.15 K and 59 MPa) and alkaline solution environment (pH = 11). The left half of the figure indicates the characteristics of the quartz-solution system after dissolution reaction, which can be vertically divided into three parts: solution, reaction transition layer, and unreacted crystal. In Fig. 10, the atomic types represented by the colors of each small ball are the same as those in Fig. 9. The right half of the figure indicates the species types present in different parts of the reaction system. The white ball represents hydrogen atoms, the red ball represents hydrogen atoms, and the yellow ball represents silicon atoms.

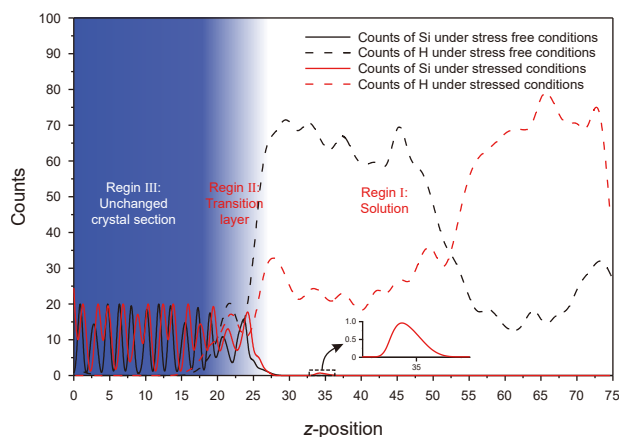


Fig. 11. Quantities distribution characteristics of hydrogen and silicon after reaction under condition of deep formation of 6000 m (442.15 K and 59 MPa) and alkaline solution environment (pH = 11).

It is generally accepted that in the lower pH range (i.e., pH < 6), the dissolution rate of quartz has little correlation with pH value (Crundwell, 2017). At higher pH values, its dissolution rate increases with the increasing of pH value (Knauss and Wolery, 1988). Within the pH range spanning acidic to alkaline conditions, the

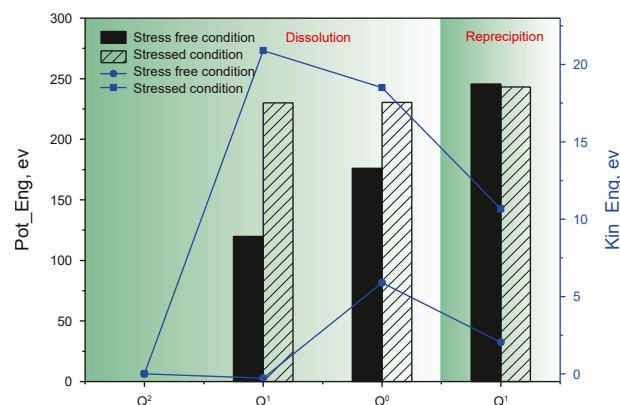


Fig. 12. Changes in system potential energy (Pot_Eng) and kinetic energy (Kin_Eng) during quartz dissolution-precipitation process (use initial state Q^2 as the reference benchmark).

dissolution mechanism of quartz may undergo significant changes (Nangia and Garrison, 2008). Previous studies have also reported an increase in the dissolution rate of quartz in acidic environments, which is mainly related to the role of organic components (Bennett and Siegel, 1987; Blake and Walter, 1999). In the present work, simulation experiments adjusted the pH environment of the

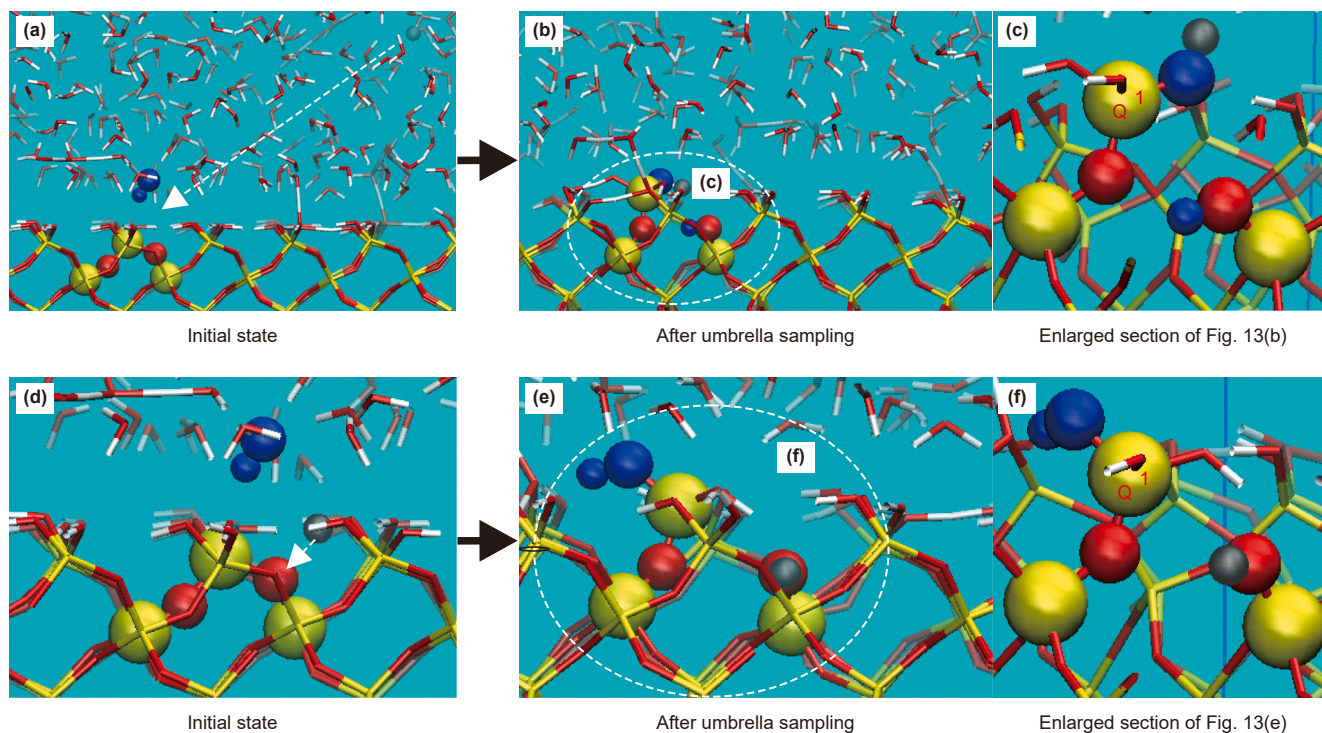


Fig. 13. Configuration of the target silicon atom at the first inflection point of the free energy curve at pH 9.5. The reaction process of Q^2 group forming Q^1 group under stress free ((a)–(c)), corresponding to the position indicated by the black arrow in Fig. 8(a)) and stressed ((d)–(f)), corresponding to the position indicated by the black arrow in Fig. 8(b)) conditions at pH 9.5. The larger blue sphere represents the oxygen in the water molecule, while the smaller blue sphere represents hydrogen in water molecules. In (a)–(c), the dark gray spheres represent hydrogen in water molecules, while in (d)–(f), the dark gray spheres represent hydrogen in hydroxyl groups on the quartz surface. (b) and (e) show the corresponding enlarged part on the right side ((c) and (f) respectively).

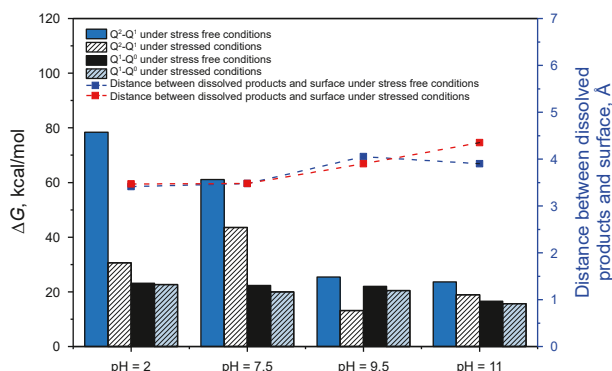


Fig. 14. Free energy barriers of key processes during Q^2 site dissolution on quartz surface in four simulated experimental environments.

system by varying the degree of deprotonation on the quartz surface. The mechanism of organic acids promoting quartz dissolution needs further exploration.

From the simulated results, it can be observed that in the two sets of simulations with $pH > 7.5$, the free energy barrier at each stage of Q^2 site dissolution exhibited a significant decrease, reflecting the promoting effect of alkaline environment on quartz dissolution, which is consistent with basic experimental knowledge and indicates the rationality of the simulated experiment. At $pH = 2$ and $pH = 7.5$, the free energy barrier of the dissolution limiting step ($Q^2 \rightarrow Q^1$) were at a high level of the four simulated environments, meanwhile, the required free energy for the $Q^1 \rightarrow Q^0$ process were of relatively smaller difference compared to the other two solution environments, indicating that the dissolution of quartz is relatively difficult in acidic and weakly alkaline environments.

In addition to analyzing the free energy barrier of key processes in the dissolution process, we also quantified the distance from the quartz surface to the first formation site of the final dissolution product ($Si(OH)_4$) in stress free and stressed environments (Fig. 14). The magnitude of the distance to some extent reflects the speed of formation of the dissolution products. A shorter distance indicates that less sampling time is required to form the final dissolution product, and the addition of stress had no significant effect on this distance. However, in alkaline environments, although the free energy barrier at each stage of Q^2 site dissolution was relatively low, the time required to form dissolution products was slightly longer than under acidic conditions, reflecting a change in the dissolution process and dissolution mechanism of quartz under acidic and alkaline solution conditions.

5.3. Influence of stress on quartz properties and latent effects of multi-factor coupling on quartz dissolution

From the data collected from thin section (Figs. 5 and 6), it can be observed that within the depth range of 7000–8000 m, the porosity of the reservoir is higher than that in adjacent depth intervals, and the proportion of quartz particle dissolution pores in secondary dissolution pores can reach over 80%, they also account for a substantial proportion of total porosity, reaching up to approximately 80%. The samples are generally subjected to high paleotectonic stress, and there is a clear positive correlation between the paleotectonic stress of the sample and the development of quartz particle dissolution pores within it (Fig. 6). This indicates that under the background of strong tectonic compression of the foreland basins, quartz dissolution induced by tectonic stress compression plays an important role in reservoir development.

From the perspective of crystal characteristics, under stressed conditions, crystals exhibit various responses, such as increased dislocation density (Kohlstedt and Weathers, 1980) and elevated strain. Dislocations are linear defects that induce lattice distortion and increase strain energy, thereby raising the internal energy of the crystal (Blum et al., 1990), this provides favorable sites for the crystal surface dissolution. The elevated strain also exerts a positive effect on crystals dissolution. Studies have shown that the dissolution rate of strained calcite crystals increases by 2–3 times compared to the original crystals (Schott et al., 1989).

The simulation experiment presented here investigated quartz dissolution based on strain, and the results showed that in an alkaline solution environment, the introduction of stress not only significantly reduced the free energy barriers of the two key processes ($Q^2 \rightarrow Q^1$ and $Q^1 \rightarrow Q^0$) (Fig. 14), but also substantially lowered the free energy barriers for the entire dissolution reaction process (Fig. 15). Through molecular simulation results, the introduction of stress conditions on the one hand increases the thickness of the reaction transition layer (Fig. 9), and the silicon content in the transition layer is significantly higher than that under stress free conditions (Fig. 11), this indicates that more silicon is about to dissolve into the solution. On the other hand, under stress conditions, the potential energy and kinetic energy of the system during the dissolution stage are higher, which suggests that dissolution occurs more easily (Fig. 12). However, in an acidic solution environment, after the addition of stress, the free energy barrier during the dissolution reaction process only slightly decreased, indicating that stress exerts a relatively weak promotional effect on the dissolution of quartz in acidic solution environments. Overall, for quartz, the stress environment can reduce the free energy barrier required for its dissolution reaction, thereby facilitating the dissolution process.

During the stratigraphic burial process, temperature gradually increases with burial depth, and studies have shown that elevated temperatures can significantly enhance the dissolution rate of quartz (Crundwell, 2017). In the geological context of foreland basins, besides the high-temperature background of deep to ultra-deep formations, tectonic stress is also an indispensable factor. As noted earlier, dislocations generated in crystals under stress conditions lead to an increase in crystal internal energy, providing favorable sites for crystal surface dissolution. Thus, in the geological setting of deep to ultra-deep formations in foreland basins, the synergistic effect of temperature and stress is of great significance for accelerating the dissolution reaction rate of quartz and creating preferential reaction sites.

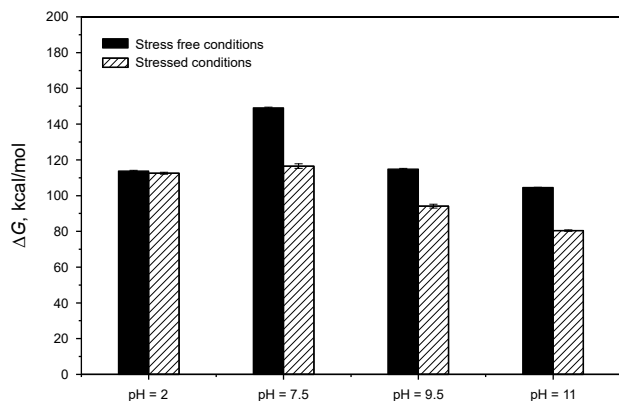


Fig. 15. Free energy change of the $Q^2 \rightarrow Q^0$ process in a simulated experimental environment.

Furthermore, under the action of tectonic stress, the number of reservoir fractures can increase, this improves fluid migration pathways, thereby facilitating the removal and supply of reactants and indirectly regulating the chemical field of the reaction. To a certain extent, the coupling of stress and chemical field is crucial for maintaining the sustainability of the reaction. In the natural water-rock reaction “laboratory” of deep to ultra-deep formations in foreland basins, the joint regulation of temperature, stress, and chemical field exerts a significant influence on the dissolution-precipitation behavior of minerals. Due to current limitations, in subsequent studies, we will focus on the dynamic response processes of mineral reaction characteristics under dynamic factors (e.g., temperature, stress, and chemical field).

5.4. Inspiration of high-quality reservoir development of foreland basin

With the advancement of oil and gas exploration, along with the development of oil and gas exploration theories and technical equipment, global deep to ultra-deep oil and gas exploration has exhibited a rapid growth trend. Developing deep basins reservoirs has become a key approach for many countries to expand oil and gas reserves. Since 2000, the number of global deep to ultra-deep oil and gas reservoirs has increased significantly (Jia and Pang, 2015; Feng et al., 2016). The secondary pores generated by dissolution are the main cause of the formation of high-quality clastic reservoirs in deep and ultra-deep intervals (Feng et al., 2016).

Reservoir spaces types in foreland basins are generally considered to be dominated by intergranular pores and micro-cracks, which mainly include residual primary intergranular pores and intergranular dissolution pores (Li et al., 2017a). Among these, intergranular dissolution pores are more commonly formed by the dissolution of unstable components such as feldspar (Stroker et al., 2013; Civitelli et al., 2023). From the diagenetic stage perspective, quartz dissolution under alkaline conditions exhibits unique stage characteristics in the context of strong tectonic compression. The special nature of quartz dissolution intensity under alkaline conditions is jointly controlled by the fluid chemical environment and molecular reaction mechanism induced by strong structural compression. When the burial depth of the reservoir exceeds 4000 m and enters the middle diagenetic stage B, organic acids are gradually consumed, the fluid pH value rises to alkaline levels, the structural compressive stress is further enhanced, and pressure dissolution between particles gradually becomes significant. Under such alkaline fluid environment and strong tectonic compression stress conditions, although tectonic compression reduces intergranular pores to a certain extent, it can provide migration channels for alkaline fluids through structural fractures, promoting the dissolution of quartz. Thin section statistical data also shows that the dissolution of quartz particles contributes a considerable amount of reservoir space (Figs. 4 and 5), laying the foundation for the formation of high-quality reservoirs. The background of multiple oil and gas charging events in the research area has become an indispensable factor in the formation of favorable industrial production capacity zones (the earliest one occurred around 14–11 Ma) (Wang et al., 2025). At the same time, molecular dynamics simulation experiments revealed that the energy barrier for quartz dissolution is lower under alkaline fluid and lateral compressive stress conditions (Figs. 8 and 14), which explains the dissolution phenomenon of quartz within the Bashijiqike Formation.

In this study, through the analysis of thin sections of the Cretaceous Bashijiqike Formation reservoir in the Kuqa foreland basin, it was found that under this strong lateral compression environment, particles are in close contact on the one hand, and on

the other hand, a large amount of extensive dissolution of quartz particles could clearly be observed (Fig. 4), and quartz particle dissolution pores accounted for a high proportion of the total pores and secondary porosity of the thin sections. This indicates that under the background of strong lateral compressive stress of the foreland basins, the pores formed by the dissolution of quartz particles play an important role in the deep reservoir space. Due to the high hardness of quartz particles, they are difficult to crush. Once secondary dissolution pores are formed during the diagenetic evolution process, they can be continuously preserved even after subsequent structural modifications, which is beneficial for expanding the exploration lower limit of deep to ultra-deep high-quality reservoirs. In this study, we mainly explored the dissolution characteristics of quartz particles under the background of strong lateral compression in foreland basins, and whether compressive stress can promote the dissolution of common minerals in reservoirs such as feldspar and carbonate minerals is also a direction that requires further research in the future.

6. Conclusion

In this study, through the combined analysis of geological samples and molecular dynamics simulations experiments, we have gained a deeper understanding of the high-quality reservoir development under strong lateral compression in foreland basins.

Through the analysis of the thin section data from the Bashiji-kike Formation, it was found that in the context of foreland basins with strong lateral compressive stress environment, mineral particles exhibit tight contact on the one hand, primarily characterized by line contact, concave-convex contact, and point contact. On the other hand, quartz particle dissolution pores also account for a high proportion of the reservoir, mainly manifested as edge dissolution and internal dissolution, and some quartz particles can have a dissolution area of more than 50%.

The results of molecular dynamics simulation experiments reveal the atomic level details of quartz dissolution under lateral compressive stress conditions, and assess dissolution difficulty from an energy perspective. During the reaction process, significant material exchange occurred between quartz and the solution, forming a transition layer on quartz surface, besides; furthermore, when stress is applied, the transition layer is thicker. Throughout the dissolution process, various types of quartz species (e.g., Q^4 , Q^3 , Q^2 , Q^1) appeared in this layer, this indicates the breakage of Si-O-Si bonds and the formation of hydroxyl groups within the layer. In the closed system of the simulation experiment, the dissolved portion of quartz eventually returned to the quartz surface and underwent reprecipitation. The application of lateral compressive stress conditions reduces the free energy barriers for the two key processes of Q^2 site dissolution on quartz surface, namely $Q^2 \rightarrow Q^1$ and $Q^1 \rightarrow Q^0$. Therefore, it plays an important role in promoting quartz dissolution; moreover, compared to acidic conditions, lateral compressive stress exerts a more significant promotional effect on quartz dissolution in alkaline solution environments. The dissolution of quartz particles under strong lateral compressive stress conditions in the foreland basins is a key genetic mechanism of high-quality deep and ultra-deep reservoirs, which is conducive to extending the exploration lower limit of high-quality deep and ultra-deep reservoirs.

CRediT authorship contribution statement

Bing Wu: Writing – original draft, Visualization, Software. **Jian Wang:** Writing – review & editing, Project administration, Funding acquisition. **Ying-Chang Cao:** Methodology, Formal analysis. **Qiang Lyu:** Investigation, Conceptualization. **Song-Qing Hu:**

Methodology, Conceptualization. **Shuang-Qing Sun:** Investigation. **Hai-Jun Yang:** Validation, Investigation.

Data availability

Data are available through Mendeley Data at <https://doi.org/10.17632/ksth274yx2.2>.

(or: <https://data.mendeley.com/drafts/ksth274yx2>).

Computer code availability

The code we used in this study to calculating free energy was from Mr. Grossfield (Grossfield, Alan, “WHAM: the weighted histogram analysis method”, version 2.0.11, http://membrane.urmc.rochester.edu/wordpress/?page_id=126), E-mail address: alan_grossfield@urmc.rochester.edu, we express our sincerest gratitude for this.

Declaration of competing interest

The authors (Bing Wu, Jian Wang, Ying-Chang Cao, Qiang Lyu, Song-Qing Hu, Shuang-Qing Sun, Hai-Jun Yang) declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.petsci.2026.01.033>.

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