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Insight into the role of masking agents in inhibiting water-based mud contamination of oil well cement slurry



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ABSTRACT

During cementing operations, unavoidable contact between water-based mud (WBM) and oil well cement (OWC) often degrades OWC performance. This is particularly problematic in natural gas or offshore wells, where zonal isolation failure can result in gas or liquid leakage, posing significant environmental and safety risks. To alleviate this problem, a masking agent was incorporated into the OWC to suppress contamination. The masking agent functions by shielding the active sites on cement particles and chelating metal ions, thereby inhibiting the cross-linking between WBM and OWC. Experimental results demonstrated that the addition of 0.5% of the masking agent increased the thickening time of the contaminated OWC system by 276%, while also doubling both its fluidity and compressive strength. To gain a more comprehensive understanding of the underlying mechanism, quantum chemistry and molecular dynamics simulations were employed. The results indicate that the masking agent exhibits superior adsorption properties, allowing it to compete effectively with the polymers for reaction sites. Overall, this study emphasizes the critical role of the masking agent in mitigating WBM contamination and proposes a viable strategy to improve the safety and quality of cementing operations. Furthermore, this approach can reduce or eliminate the need for spacer fluids, thereby addressing environmental challenges associated with the disposal of wellbore waste fluids.

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1. Introduction

Oil and gas exploration and development are advancing into increasingly complex and extreme environments, with the drilling of unconventional oil and gas, such as deep and ultra-deep wells, becoming a key method for accessing deep oil and gas resources. Water-based mud (WBM), as a critical fluid in drilling engineering, consists of bentonite, various polymer agents (such as diluents, fluid loss additives, encapsulants, and shale inhibitors), and weighting materials (Guo et al., 2024; Huang et al., 2018; You et al., 2025; Zhang et al., 2024c). To maintain stability and functionality under extreme conditions, WBM formulations have become

increasingly complex, posing significant challenges to the performance of oil well cement (OWC) during subsequent cementing operations (Huang et al., 2023; Liu et al., 2020; Noor et al., 2025). Due to the complex composition of WBM, contact with cement slurry often leads to degradation of slurry properties, mainly manifested as shortened thickening time, abnormal gelation, abnormal thickening, and a decrease in compressive strength (Dehvedar et al., 2025; Zhang et al., 2021a). At the same time, the sealing integrity between the cement annulus and the formation will be compromised (Bu et al., 2020a, 2020b; Katende et al., 2020; Lian et al., 2023). Especially in gas wells and offshore oil and gas well cementing operations, failure in zonal isolation can create migration channels for gas or liquids, leading to methane or drilling fluid leakage, which will cause serious environmental and marine pollution issues (Kiran et al., 2017; Mohammed et al., 2019; Su et al., 2021; Yu et al., 2024). In severe cases, this may lead to cementing failures such as casing blockage, annular bridging, or the inability to retrieve the drill string or tubing after cementing.

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To address WBM contamination, existing solutions primarily rely on increasing the volume of spacer fluids or adding high-dose retarders to extend the thickening time of the contaminated cement slurry (Moradi et al., 2020; Salimi et al., 2024; Zhang et al., 2024a). However, these approaches do not fundamentally address contamination. In practical cementing operations, the displacement efficiency of spacer fluids and flushing fluids rarely reaches 100%, leading to potential contamination between the OWC and WBM (Alkhalaf et al., 2023; Wu et al., 2024b). Furthermore, the extensive use of spacer fluids and retarders also increases costs. While “pilot slurries” (WBM with reduced additive content) are used on-site to minimize contamination, this approach has critical flaws. The stability of the pilot slurry is compromised by reduced polymer content, particularly at high temperatures, weakening its overall stability and increasing the risk of cementing failure. Therefore, implementing measures at the OWC-WBM interface is the fundamental approach for achieving contamination resistance.

Currently, the primary field methods for mitigating WBM contamination in cement slurries involve adjusting mud formulations or employing spacer fluids. However, the subsequent treatment of returned spacer fluids and pilot slurries remains a significant challenge (Deng et al., 2024; Yang et al., 2023a). As energy strategies shift towards sustainable development, environmental requirements for oil and gas extraction have become more stringent. The treatment of such waste fluids requires pH neutralization, polymer degradation using ammonium persulfate oxidants or gel breakers, and subsequent testing for chemical oxygen demand (COD), biochemical oxygen demand (BOD), and heavy metal content (Guo et al., 2013). Only when they meet national standards can these fluids be discharged (Kazamias and Zorpas, 2021). Discharging wellbore waste fluids not only incurs substantial financial costs but also exerts immense pressure on environmental protection efforts. Consequently, reducing waste fluids is the optimal anti-contamination strategy.

To minimize waste liquid emissions and enhance anti-contamination performance, the masking agent DTPMPA was introduced into the cement slurry in this study. The advantage of DTPMPA lies in its molecular structure, which contains five phosphonic acid groups capable of forming stable, multi-dentate, multimetal chelation structures with active sites in the cement slurry (Cardiano et al., 2017; Nouigues et al., 2024; Zeino et al., 2018). In addition, molecular dynamics (MD) and density functional theory (DFT) simulations were employed to analyze how the functional groups of DTPMPA influence adsorption strength, characterizing its adsorption configurations and bonding modes on cement mineral surfaces in terms of energy and conformation (Chen et al., 2023; Wu et al., 2024a). Compared to other phosphonates (such as ATMP or HEDP), DTPMPA exhibits a higher chelation capacity for calcium, aluminum, and iron ions (Lv et al., 2022; Rabizadeh et al., 2020; Zeino et al., 2018). Additionally, its excellent thermal stability ($>210^{\circ}\text{C}$) makes it highly suitable for high-temperature cement slurry systems that encounter drilling fluid contamination at low dosages (Long et al., 2026).

This research evaluates the anti-contamination efficacy of the masking agent, without the use of spacer fluids or pilot slurries. The focus of this research differs from the traditional “passive resistance” approach to anti-contamination strategies. We propose, for the first time, introducing the “masking agent” DTPMPA into the cement slurry to achieve “active interception” of WBM, which represents a preventive control strategy. Furthermore, the study elucidates the competitive adsorption behavior between DTPMPA and WBM additives on the hydration surfaces of cement minerals and metal ions, directly revealing the microscopic mechanism by which the masking agent occupies and competes

for adsorption sites. A multiscale, closed-loop research system was established, spanning from simulated calculations of molecular functional group characteristics (the strong chelation ability of DTPMPA's polyphosphonic acid groups) to competitive adsorption experiments, and ultimately to the verification of microstructure and macroscopic performance. This provides robust evidence of the effectiveness of “chemical masking”. Further deepening our understanding of strategies for controlling OWC contamination caused by WBM contact.

2. Materials and methods

2.1. Experimental materials

In this experiment, Class G oil well cement was sourced from Jiahua Special Cement Co., Ltd. The cement slurry additives, including retarder HX-36L and fluid loss agent HX-12L, were provided by OMAX Oilfield Technology Co., Ltd. The WBM and related treatment agents were obtained from an oilfield in Xinjiang, China. The small molecule DTPMPA was purchased from Shanghai Aladdin Biochemical Technology Co., Ltd.

Tricalcium silicate (C_3S) was synthesized in the laboratory using raw materials of CaCO_3 , SiO_2 , Al_2O_3 , and MgO , all purchased from Shanghai Aladdin Biochemical Technology Co., Ltd. The synthesis conditions are listed in Table S1. Particle size analysis was conducted on the synthesized C_3S clinker phase, and the results are shown in Fig. S1.

2.2. Experimental methods

2.2.1. Sample preparation

Following the procedure in API RP 10B (2013), the cement slurry was mixed with WBM to facilitate the analysis and comparison of the experimental results.

The composition of the cement slurry is shown in Table S2, while the main components of the WBM are listed in Table S3. The cement slurry contamination process involved replacing a portion of the slurry with WBM. Cement slurry and WBM were blended with the OWC-9360 constant-speed mixer from the Applied Technology Research Institute at Shenyang Aerospace University.

2.2.2. Sample testing

The rheological parameters of the cement slurry were measured using a ZNN-D12B rotational viscometer in accordance with the API RP 10B procedures. Fluidity was determined by averaging the maximum diameters of the slurry spread in two perpendicular directions using a small slump cone. In accordance with API RP 10B, cement slurry samples were prepared and subsequently cured at a bottomhole static temperature (BHST) of 160°C and a pressure of 20.7 MPa for durations of 24, 48, and 168 h, respectively. After curing, the samples were demolded and cooled to ambient temperature. Compressive strength was evaluated using an OWC-2002 oil well cement pressurizing machine (Shenyang Aerospace University); for each condition, five replicates were tested to calculate the average value. Additionally, thickening time tests were conducted at 160°C and 70 MPa for 90 min using an OWC-9480C high-temperature and high-pressure (HTHP) consistometer (Applied Technology Research Institute, Shenyang Aerospace University) according to API RP 10B specifications.

2.2.3. Characterization

The zeta potential analyzer (Zeta Probe, USA) was used to detect the zeta potential of the C_3S after adding DTPMPA and

sulfonated filtrate reducer (KLS). At 25 °C, a slurry was prepared by mixing 10 g of C₃S, 100 g of water, and a predetermined amount of chemical additives, with the pH adjusted to 13, similar to the chemical environment of cement slurry (Zhu et al., 2018, 2021). To monitor the variation in zeta potential under stable conditions of the cement slurry, the zeta potential was measured every 5 s, and the average value was taken.

Liquid nitrogen freeze-drying was used to arrest cement hydration at various time intervals. Samples were removed after curing in a constant-pressure water bath at 90 °C for 10 min, 180 min, and 2 d. Afterward, the samples were frozen with liquid nitrogen for 5 min and vacuum-dried for 2 d. In the experiment, a Zeiss Sigma 300 scanning electron microscope (SEM) was used to observe the microstructure of the cement slurry. Due to the low conductivity of cement, samples were sputter-coated with gold to enhance imaging quality. X-ray diffraction (XRD) analysis of the powdered samples was performed using a Thermo Fisher Scientific XRD with Cu K α radiation. Data were collected over the 2 θ range from 5° to 90° at a scanning speed of 5°/min. The obtained data were analyzed using the Crystallography Open Database (COD).

Isothermal calorimetry (TAM-Air) was employed to measure heat release and heat release rate during cement hydration. The experimental samples were prepared by mixing water and a cement slurry at a water–cement ratio (W/C) of 0.44, and the heat release during the cement hydration was continuously monitored over 72 h at 20 °C. To prepare the sample for analysis of the chemical adsorption state, 1 g of C₃S was separately dispersed in 100 mL of solutions containing 1% concentrations of DTPMPA and KLS. After stirring for 10 min, the cement particles were filtered, washed, and dried in a vacuum oven to obtain the final sample for X-ray photoelectron spectroscopy (XPS) analysis (Feng et al., 2024; Guo et al., 2017). XPS analysis was conducted on a Thermo scientific instrument equipped with a monochromatic Al K α source (1486.6 eV), using a 400 μ m spot size and an operating voltage of 12 kV. Before peak fitting, the spectra were preprocessed using the Shirley method for background subtraction. The binding energy of XPS spectra was calibrated with the C 1s band at 284.8 eV. The peak shape was fixed with 80% Gaussian–20% Lorentzian, and the fullwidth half-max (FWHM) was allowed to vary for each individual peak.

The metal ions in the samples were analyzed using an Agilent 720 ES inductively coupled plasma optical emission spectrometer (ICP-OES). The cement paste filtrate was collected after curing at 90 °C for 20 min, then centrifuged at 4000 rpm for 10 min, and then diluted tenfold.

2.3. Simulation methods

2.3.1. Quantum chemistry simulation

Density functional theory (DFT) calculations were performed using the DMol3 and CASTEP modules in Materials Studio to analyze molecular charge distributions and their variations on the C₃S surface (Claverie et al., 2019; Li et al., 2022). The generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional was employed, and a double numerical plus polarization (DNP) basis set was selected. The convergence criteria for energy, maximum force, and displacement are set to 2×10^{-5} Ha, 4×10^{-3} Ha/Å, and 5×10^{-3} Å, respectively. The self-consistent field (SCF) tolerance was set at 1×10^{-5} Å. A smear value of 0.005 Ha was fixed throughout the calculations. The DTPMPA molecule (Fig. 1(a)) and KLS polymer fragment (Fig. 1(b)) were modeled based on their established structures. According to the analysis by Mishra et al. (2013a), over 20 different (*hkl*) cleavage planes, organic additives preferentially

adsorb on the energy-stable (040) plane, which has the lowest cleavage energy. Therefore, the (040) surface was selected for subsequent research (Chaudhari et al., 2017; Mishra et al., 2013a). This surface was modeled using a $2 \times 1 \times 1$ supercell with a 25 Å vacuum layer along the *c*-axis to prevent periodic interactions. The C₃S crystal CIF file was sourced from the American Mineralogist Crystal Structure Database and optimized using the CASTEP module in Materials Studio. To verify the accuracy of the model, simulated XRD patterns were compared with experimental data (Fig. 1(c)). The high degree of consistency confirmed that the model met the required accuracy. Finally, the initial interfacial configurations of KLS (polymer fragment) and DTPMPA on the C₃S (040) plane prior to geometry optimization are illustrated in Fig. 1(d, e) (Claverie et al., 2019; Wang et al., 2018).

2.3.2. Molecular dynamics simulations

All molecular dynamics (MD) simulations were conducted using the Forcite module in Materials Studio (Li et al., 2017; Miao et al., 2025). The simulation system consists of DTPMPA, KLS polymer fragment, water, and metal ions in the cement slurry. The molecular model underwent pre-optimization using the Dmol3 module, with model parameters refined using the GGA–PBE/DNP functional, and charges were determined using the charge balance method (QEq). As deprotonation occurs for groups in the polymer and DTPMPA in the alkaline cement slurry, Na⁺ and Cl[−] ions are added to balance the charges (Wilson et al., 2021). The specific components of the three solution models are detailed in Table 1.

The lattice parameter and atomic positions were optimized using the Forcite geometry optimization module with the Smart algorithm. The convergence tolerances for energy, force, and displacement were set to 2×10^{-5} kcal/mol, 1×10^{-3} kcal/(mol·Å), and 1×10^{-5} Å, respectively. The solution box model was created using the Amorphous Cell module, and the structure and properties were calculated using the COMPASS II force field. The dynamic simulation parameters for the solution models are presented in Table S4. Based on the component parameters in Table 1, the initial configurations of three solution models were constructed, as shown in Fig. 1(f–h).

3. Results and discussion

3.1. Analysis of contamination

3.1.1. Macroscopic analysis

Based on the proportions recommended by API RP 10B (2013), mixtures were prepared at cement slurry: WBM blending ratios of 100:0, 90:10, 80:20, 70:30, and 50:50. The influence of WBM on the flowability, compressive strength, and thickening time of the cement slurry was investigated.

As illustrated in Fig. 2(a), the compressive strength of the cement slurry decreased as the blending ratio of WBM increased. At a 50:50 blending ratio, the cement slurry did not solidify even after 7 d of curing. Fig. 2(b) shows that increasing the WBM proportion in the cement slurry significantly reduced its flowability. At a 70:30 ratio, the cement slurry exhibited complete loss of fluidity after curing at high temperatures for 20 min. Interestingly, at a 50:50 ratio, the flowability of the contaminated cement slurry improved, likely due to a reduction in solid particles. Thickening experiments were conducted on cement slurries with different blending ratios of contaminated WBM (Fig. 2(c)). With the addition of WBM, the contaminated cement slurry exhibited abnormal gelling phenomena regardless of the blending ratio. At a 70:30 blending ratio, the thickening time was decreased to 93 min, and the consistency curve showed abnormal thickening.

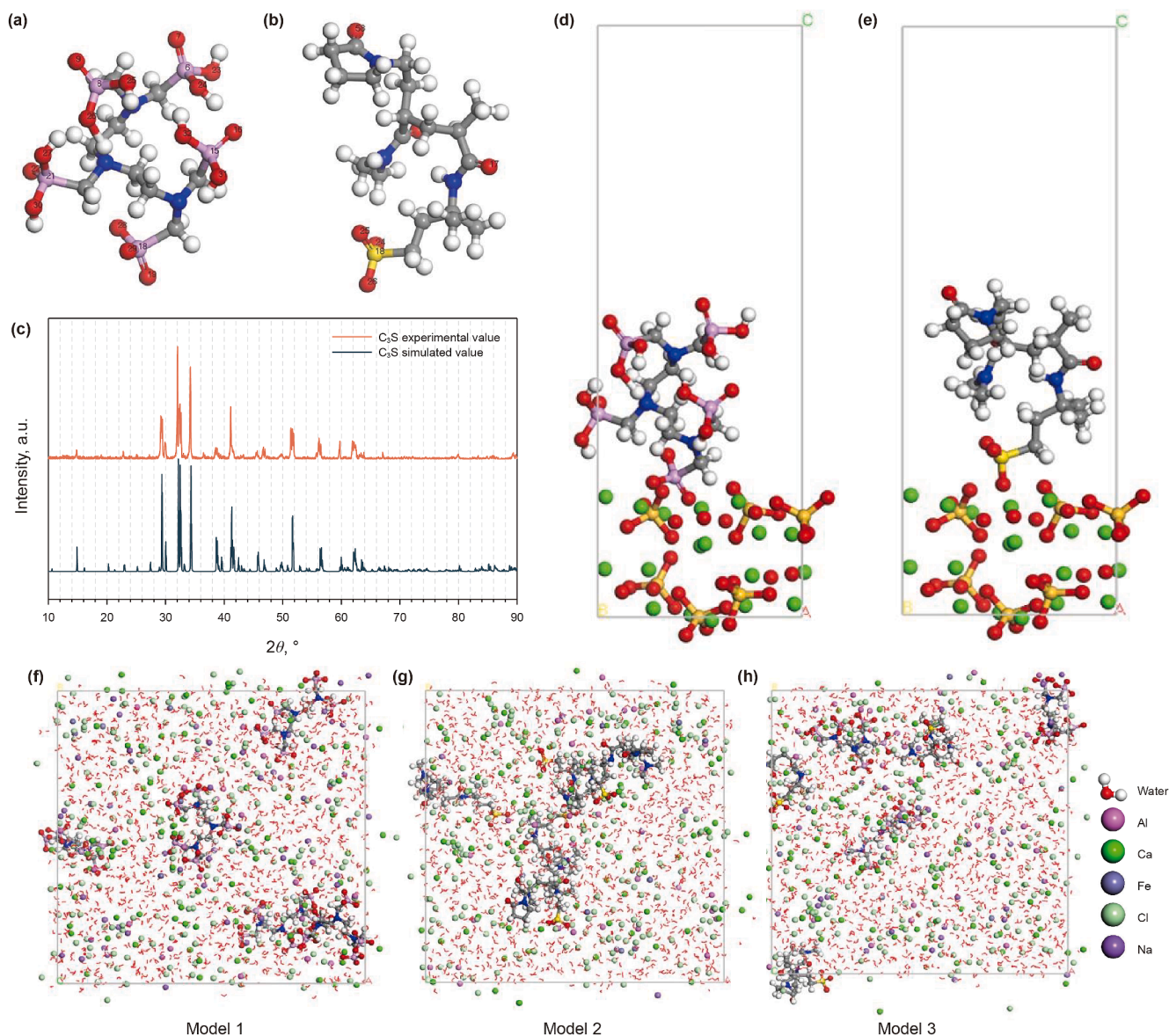


Fig. 1. Initial models. (a) DTPMPA; (b) KLS polymer fragment; (c) XRD pattern of C_3S crystal; (d) DTPMPA/ C_3S composite; (e) KLS polymer fragment/ C_3S composite; (f–h) initial configurations of three models of metal ions and molecular solutions.

Table 1
Composition of the solution model.

Type	Water	Fe ³⁺	Al ³⁺	Ca ²⁺	Na ⁺	Cl [−]	DTPMPA	KLS
Model 1	1500	10	30	100	5	220	0	5
Model 2	1500	10	30	100	50	220	5	0
Model 3	1500	10	30	100	33	220	3	3

Due to the complexity of WBM, mixing it with cement slurry does not fully reveal the contamination mechanism. As a result, it is crucial to simplify the problem and adopt a single-factor approach to examine the effects of WBM additives on the flowability and compressive strength of the cement slurry. This will help identify the most severe contaminants. In this study, three representative types of polymer additives in WBM were investigated: fluid loss additive (KLS) (Li et al., 2024), lubricant (YRH) (Yang et al., 2023b), and blocking agent (YFT) (Li et al., 2025).

Based on different blending ratios of cement slurry and WBM, the 70:30 blend was identified as the most severe contamination level. Therefore, the WBM additives were added to the slurry at a 70:30 blending ratio, with dosages in WBM as follows: KLS at 1%, YRH at 3%, and YFT at 3%. After contamination with a single additive, the compressive strength of the cement pastes was significantly reduced (Fig. S2(a)). Among them, KLS has the greatest impact on cement slurry contamination. With just a 1% addition, the compressive strength of the cement paste drops from 21 MPa at 3 d to 0 MPa. As shown in Fig. S2(b), after being cured at 90 °C for 20 min, the cement slurry loses its fluidity and becomes more elastic. As shown in Fig. S3(a), FTIR spectroscopy revealed that the characteristic peak of the KLS polymer at 3431 cm^{-1} corresponds to $-\text{OH}$, peaks at 2923 and 2855 cm^{-1} are attributed to the asymmetric and symmetric stretching vibration of methylene groups. The peak at 1630 cm^{-1} represents the carbonyl ($\text{C}=\text{O}$) stretching vibration of amide groups. The peak at 1443 cm^{-1} is attributed to the bending vibration of methylene groups, while the

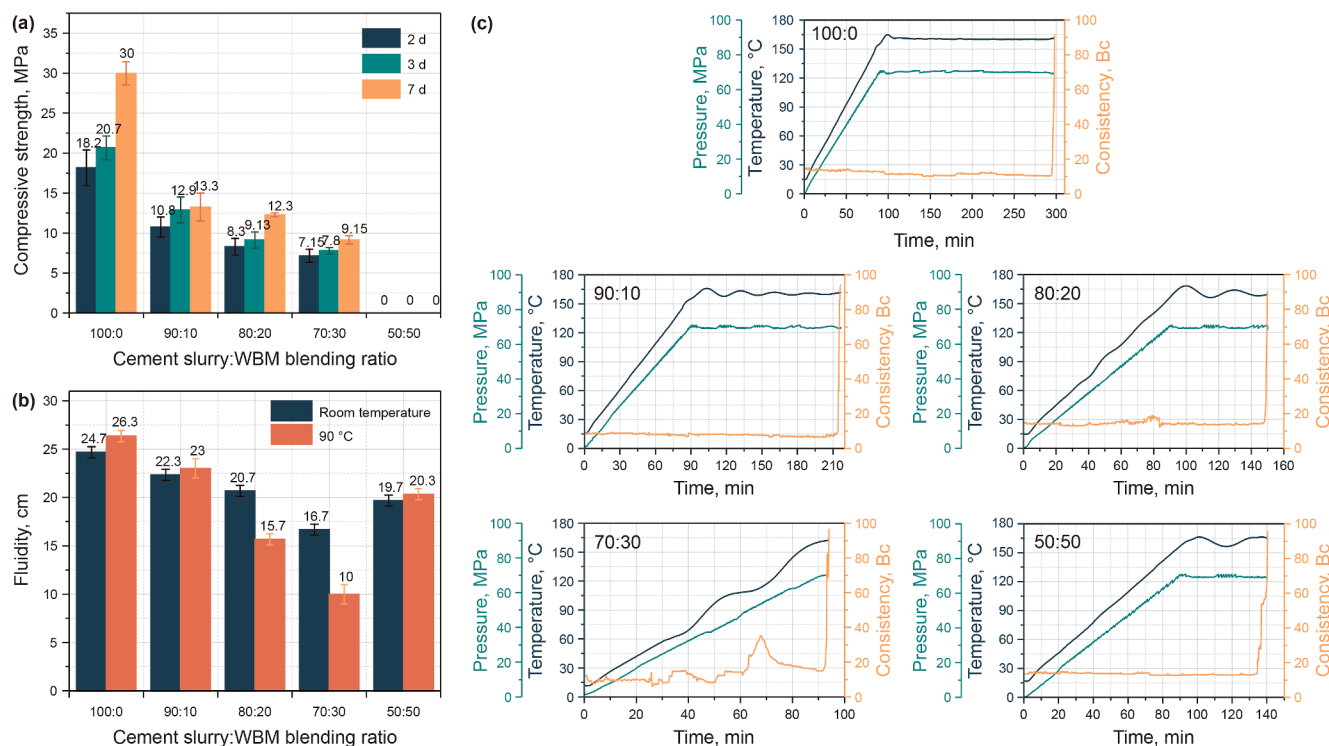


Fig. 2. Performance of cement slurry under different blending ratios with WBM. (a) Compressive strength; (b) fluidity; (c) thickening experimental results.

peak at 1328 cm^{-1} corresponds to the S=O stretching vibration, which is relatively weak. The characteristic peaks at 1121 and 1041 cm^{-1} are related to C–N, and the peak at 589 cm^{-1} corresponds to the out-of-plane bending vibration of C–H. The molecular weight and distribution of the KLS polymer were determined by gel permeation chromatography (GPC). The number average molecular weight (M_n) of KLS is 278,100 Da, the weight average molecular weight (M_w) is 606,811 Da, and the polydispersity index (PDI) is 2.18199 (Fig. S3(b)). Structurally, KLS is a high-molecular-weight anionic polymer synthesized via the copolymerization of 2-acryloylamino-2-methyl-1-propanesulfonic acid (AMPS), *N,N*-dimethylacrylamide (NNDMA), and *N*-vinyl-2-pyrrolidone (NVP) (Fig. S4).

Given that polymer KLS significantly impairs fluidity, it is necessary to study its interactions with both active cement particles and inert solid materials in the slurry to identify the primary cause of the decline in flowability. This study investigated the effects of different KLS dosages (0, 0.25%, 0.50%, 0.75%, and 1.00%) on the flowability of pure cement and quartz sand mortar systems at a W/C of 0.5. The results in Fig. 3(a) indicate that the rheological behavior of the cement slurry is significantly affected by varying KLS dosages. However, when the dosage reaches 1.00%, the contamination level decreases. Furthermore, Fig. 3(b) shows that in the inert quartz sand mortar system, KLS increases viscosity only marginally, regardless of the dosage. The flowability results for the cement slurry and quartz sand systems are shown in Fig. 3(c). The flowability trends of both systems are similar to those of the viscosity. Compared with the quartz sand system, the increase in viscosity in the cement slurry system is more pronounced, suggesting that the number of hydrogen bonds may not be the primary reason for the rapid increase in plastic viscosity in the cement system. Instead, the dominant factors are electrostatic interactions with dissolved ions and polymer–particle bridging. At the same time, hydrogen bonding plays a secondary role. In

contrast, in the inert quartz sand system, the low concentration of dissolved ions reduces the likelihood of polymer–particle bridging, leading to a relatively higher contribution from hydrogen bonding.

Furthermore, when the KLS dosage in the cement slurry reaches 1.00%, the plastic viscosity begins to decrease. This can be attributed to the aggregation of KLS polymers into multimeric clusters that exhibit a microgel-like structure, prone to film formation. When adsorbed onto the surfaces of two or more cement particles, they bridge the particles through electrostatic and van der Waals forces, thereby increasing slurry viscosity. However, beyond the saturation dosage, excess polymers form multilayered films due to intermolecular hydrogen bonding between polymer chains. This also means that at higher concentrations, KLS molecules adsorbed on one cement particle may fail to find available adsorption sites on another particle, thereby reducing slurry viscosity.

From another perspective, the bridging effect of polymers with long main chains (molecular weight) in KLS solutions may be the key. Cross-linking and complexation reactions typically occur between metal ions such as Ca^{2+} , Fe^{3+} , Al^{3+} , and the $-\text{SO}_3^-$ groups in the KLS (Bey et al., 2014). The experiments revealed that the addition of Al^{3+} to the KLS solution resulted in the immediate formation of a white translucent gel, which became more structured with increasing Al^{3+} concentration (Fig. 3(d)). Upon adding Fe^{3+} to the KLS, a large amount of reddish-brown translucent gel formed, which also became opaque and more structured with increasing Fe^{3+} concentration (Fig. 3(e)). In contrast, the addition of Ca^{2+} to the KLS did not cause any noticeable changes (Fig. 3(f)).

The experimental results revealed that Al^{3+} and Fe^{3+} readily form gel structures with KLS, whereas Ca^{2+} does not under the same conditions. This disparity could be attributed to the larger ionic radius and relatively lower coordination number of Ca^{2+} compared to Al^{3+} and Fe^{3+} , resulting in lower charge density. In contrast, Al^{3+} and Fe^{3+} , with higher charge density, smaller ionic

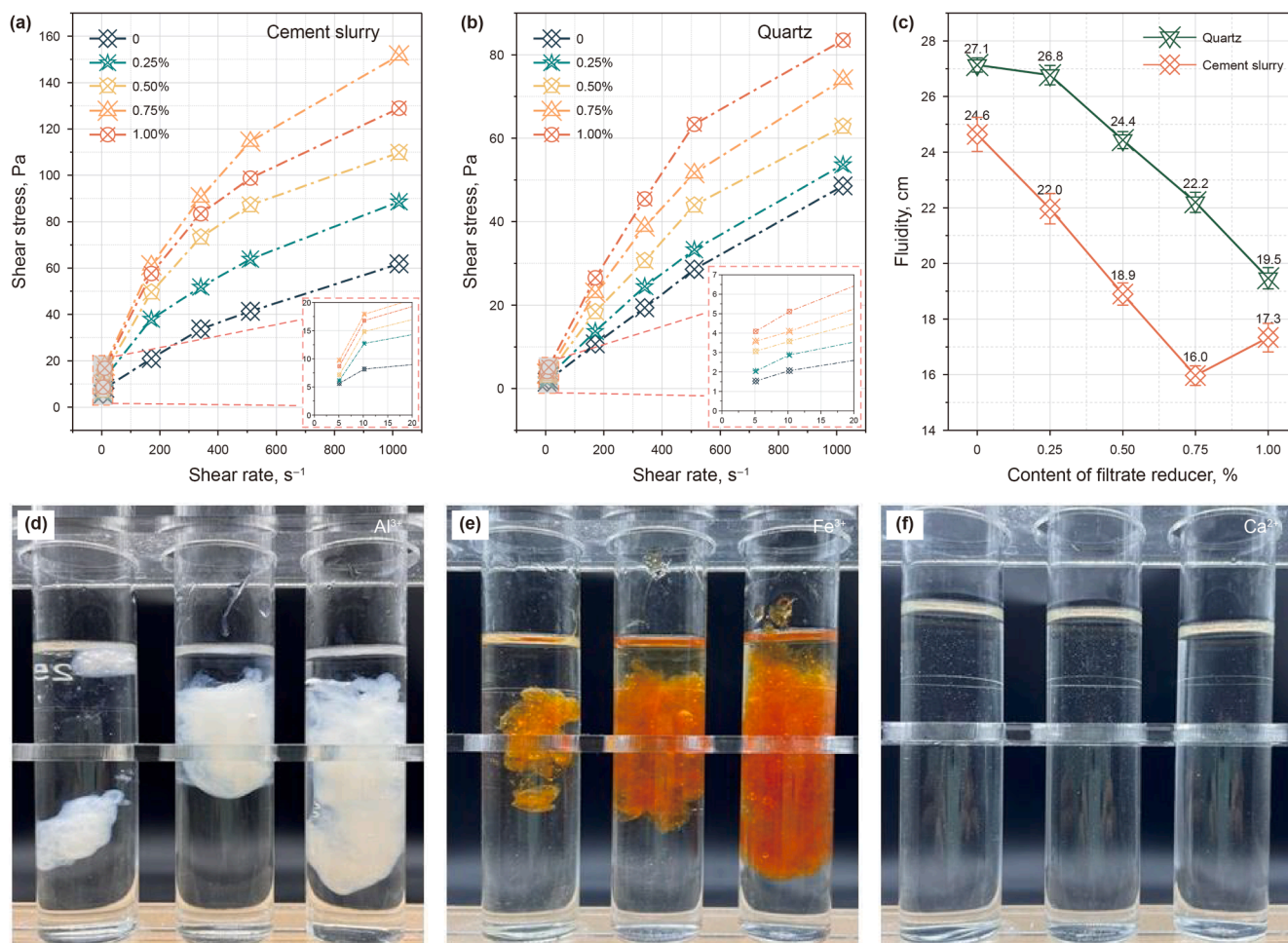


Fig. 3. Adsorption behavior of KLS with multivalent metal ions (Al^{3+} , Fe^{3+} , and Ca^{2+}) and particles. **(a, b)** Rheological curves of different dosages of the KLS in the cement slurry system and quartz sand system; **(c)** flowability of different dosages of the KLS; **(d–f)** cross-linking and complexation reactions of metal ions (Al^{3+} , Fe^{3+} , and Ca^{2+}) in the KLS solutions at concentrations of 100, 300, and 500 mg/L (from left to right).

radii, and larger coordination numbers, exhibit greater Lewis acidity, facilitating simultaneous interactions with multiple coordination sites between polymer chains and forming strong cross-linking and gel structures (Adelnia et al., 2023; Chen et al., 2022).

3.1.2. Microscopic analysis

The purpose of studying the microstructure of cement slurry is to better understand its macroscopic properties. As illustrated in Fig. 4(a), after curing at 90 °C for 180 min and subsequent freeze-drying with liquid nitrogen, microscopic analysis reveals the abundant formation of flake-like calcium hydroxide (CH) and rod-like ettringite (AFt) in normal hydrated cement (Li et al., 2021b; Sha et al., 2022). After 2 d of curing, as depicted in Fig. 4(b), significant quantities of needle-like calcium silicate hydrate (CSH) were generated (Wang et al., 2020; Zhang et al., 2017). In contrast, in the KLS-contaminated samples, a network-like structure was formed on the surface of the cement particles, cross-linking the cement particles together (Fig. 4(e)). After 2 d of hydration, no CSH was formed, which is inconsistent with regular cement hydration (Fig. 4(f)). Furthermore, elemental mapping analysis of the sample surface indicated that the middle parts were enriched with carbon and oxygen elements, accounting for more than 80% of the total, while the content of aluminum, silicon, and calcium elements remained low. These results confirm that

organic substances have enveloped the cement particles, thereby hindering the normal hydration process (Li et al., 2021a).

XRD analysis was used to identify the crystalline phases of cement hydration products and unhydrated clinker phases, along with their relative content (Sun et al., 2022; Yang et al., 2024a). This helps to accurately understand the different crystalline substances and their quantities generated during cement hydration. In this study, diffraction peaks representing tricalcium silicate (C_3S), dicalcium silicate (C_2S), tricalcium aluminate (C_3A), and CH were observed. As shown in Fig. 4(c), after 2 d of hydration, strong characteristic peaks of CH were observed, indicating a high content. Compared to cement clinker, the diffraction intensities of C_3A , C_3S , and C_2S significantly decreased or disappeared entirely (Luo et al., 2024). In Fig. 4(g), the XRD patterns of the KLS-contaminated cement slurry revealed that the polymer inhibited hydration. After 2 d of hydration, the characteristic peaks of C_3A , C_3S , and C_2S also remained, with little change in peak intensity. The Rietveld refinement was performed using Highscore software to achieve precise quantification of crystal phase development. The original curve and the fitting residuals are shown in Fig. S5. The quantification results indicate that after normal hydration of the cement slurry for 2 d, the proportion of C_3S decreased to 58.3% (relative proportions between crystal phases), while the proportion of the hydration product CH increased to 31.6% (Fig. 4(d)). After the addition of KLS to the cement slurry, the proportion of

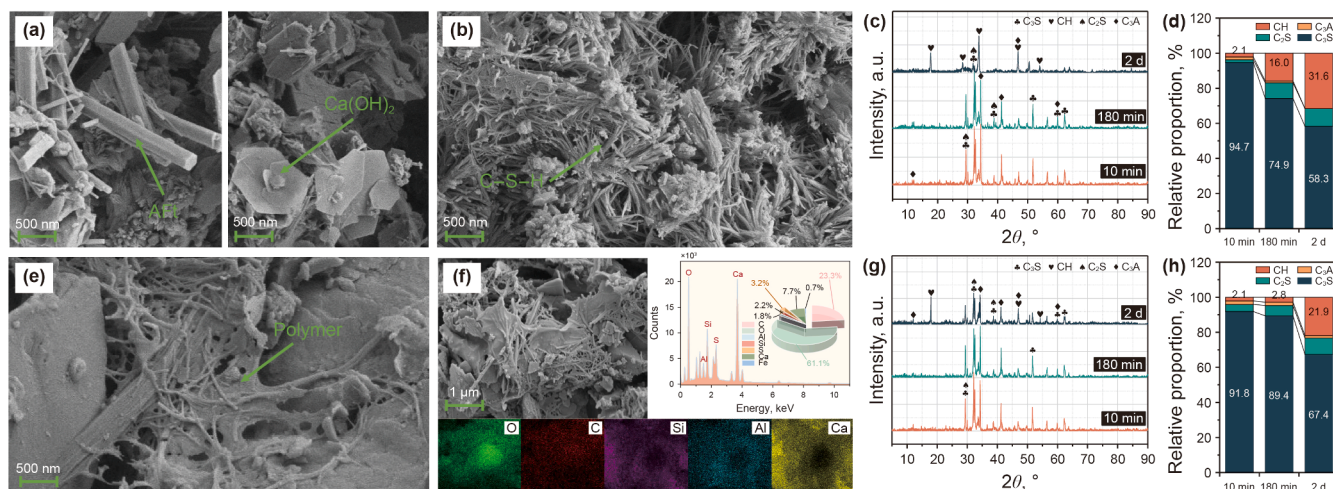


Fig. 4. Micromorphology and structural analysis of cement slurry without (a–d) and with (e–h) KLS. Control group: (a) SEM image after 180 min of hydration; (b) SEM image after 2 d of hydration; (c) XRD patterns at different hydration periods; (d) crystal phase distribution. KLS-added group: (e) SEM image after 180 min of hydration; (f) SEM image after 2 d of hydration; (g) XRD patterns at different hydration periods; (h) crystal phase distribution.

C₃S decreased to 67.4%, while CH was at 21.9% (Fig. 4(h)). Therefore, XRD analysis indicates that KLS has a significant negative effect on the normal hydration of the cement slurry, leading to hindered hydration and reduced compressive strength.

The differences in microstructure and morphology mentioned above are the main reasons for the deterioration of cement compressive strength and flowability. This can be attributed to the macromolecular structure and strong adsorption properties of KLS, which form a network-like cross-linking structure between cement particles, hindering the normal flow and hydration of the cement slurry.

3.2. Competitive adsorption mechanism investigation

In summary, based on the mechanistic analysis of contamination, an effective measure has been developed to prevent KLS and other polymers from contaminating cement slurry. The principle of the masking measure can be summarized as competitive adsorption and structure disruption. Competitive adsorption involves using small molecules with strong adsorption capacity, such as organic phosphonic acid (DTPMPA), to compete with KLS for adsorption sites on cement particles and metal ions, thereby preventing chemical reactions between polymers and cement. Since the masking agent (DTPMPA) is a small organic molecule with multiple adsorption sites, it predominantly adsorbs onto individual cement particles or forms multidentate chelates with metal ions, thereby minimizing its potential to cross-link adjacent cement particles. The goal of structural disruption is to dismantle the gel structure that has already formed between the polymers and cement particles.

3.2.1. Adsorption behavior of polymers and masking agents on the surface of clinker C₃S

The hydration of cement is significantly more complex than the sum of individual clinker hydration reactions. To further determine the reaction mechanism between masking agents, polymers, and cement clinkers, XPS analysis was performed to investigate the adsorption mechanisms of masking agents and KLS on C₃S, the most abundant single clinker in cement composition (Black et al., 2003). The O 1s spectrum of tricalcium silicate can be decomposed into four curves at 530.14, 530.94, 531.79, and 532.59 eV, corresponding to Ca–O, C–O, C=O, and Si–O, respectively (Fig. 5(a)). The

peaks of C–O and C=O may originate from carbon dioxide contamination during sample preparation.

Fig. 5(b) shows the XPS spectra of KLS before and after adsorption on C₃S. In the high-resolution O 1s spectra, a peak corresponding to the S–O bond in the sulfonic acid group is observed, with a 0.33 eV shift after adsorption. Similarly, in the O 1s spectra of DTPMPA before and after reaction, a peak originating from the P–O bond in the phosphonic acid group shows a shift of 0.53 eV (Fig. 5(c)). In the S 2p spectrum of KLS, the characteristic peak of S–O is located at 168.74 eV, while in the P 2p spectrum of DTPMPA, the characteristic peak of P–O appears at 134.25 eV. After reaction with C₃S, these characteristic peaks shift significantly by 1.05 and 1.24 eV, respectively. Fine spectral analysis of Ca 2p was performed on C₃S after KLS adsorption (Fig. 5(b)). The characteristic peaks of Ca 2p_{3/2} and Ca 2p_{1/2} are observed in the post-adsorption spectrum. Compared to the XPS spectrum of pristine C₃S (Fig. 5(a)), the shifts in the Ca 2p_{3/2} and Ca 2p_{1/2} peaks after KLS adsorption are 0.20 and 0.12 eV, respectively. In contrast, for DTPMPA adsorbed on C₃S (Fig. 5(c)), the shifts are 0.51 and 0.49 eV, respectively. The larger shift in Ca 2p binding energy after DTPMPA adsorption compared to that after KLS adsorption indicates stronger chemical adsorption of DTPMPA on the C₃S surface. The specific parameters of the adsorption behavior of KLS and DTPMPA on the C₃S surface are shown in Table 2.

To investigate the changes in surface charge of cement clinker phases before and after the adsorption of polymers and small molecules, zeta potential analysis was conducted (Fig. 5(d)). After the addition of KLS and DTPMPA to the C₃S dispersion, the zeta potential of the clinker phase in water shifted to negative values.

The positive surface charge of C₃S promotes the adsorption of negatively charged functional groups from KLS and DTPMPA onto the C₃S surface. The experiments also revealed significant differences in the adsorption behavior of KLS and DTPMPA. Within the same time frame, the change in surface charge following DTPMPA adsorption onto C₃S was more pronounced than that following KLS adsorption. During the first 15 min, the zeta potential of C₃S decreased more rapidly after DTPMPA adsorption than after KLS adsorption. When the dosages of KLS and DTPMPA were increased, the zeta potential of the clinker dispersion became even more negative. These results demonstrate that both the adsorption amount and adsorption rate of DTPMPA on the C₃S surface are significantly higher than those of KLS. This is likely due to DTPMPA

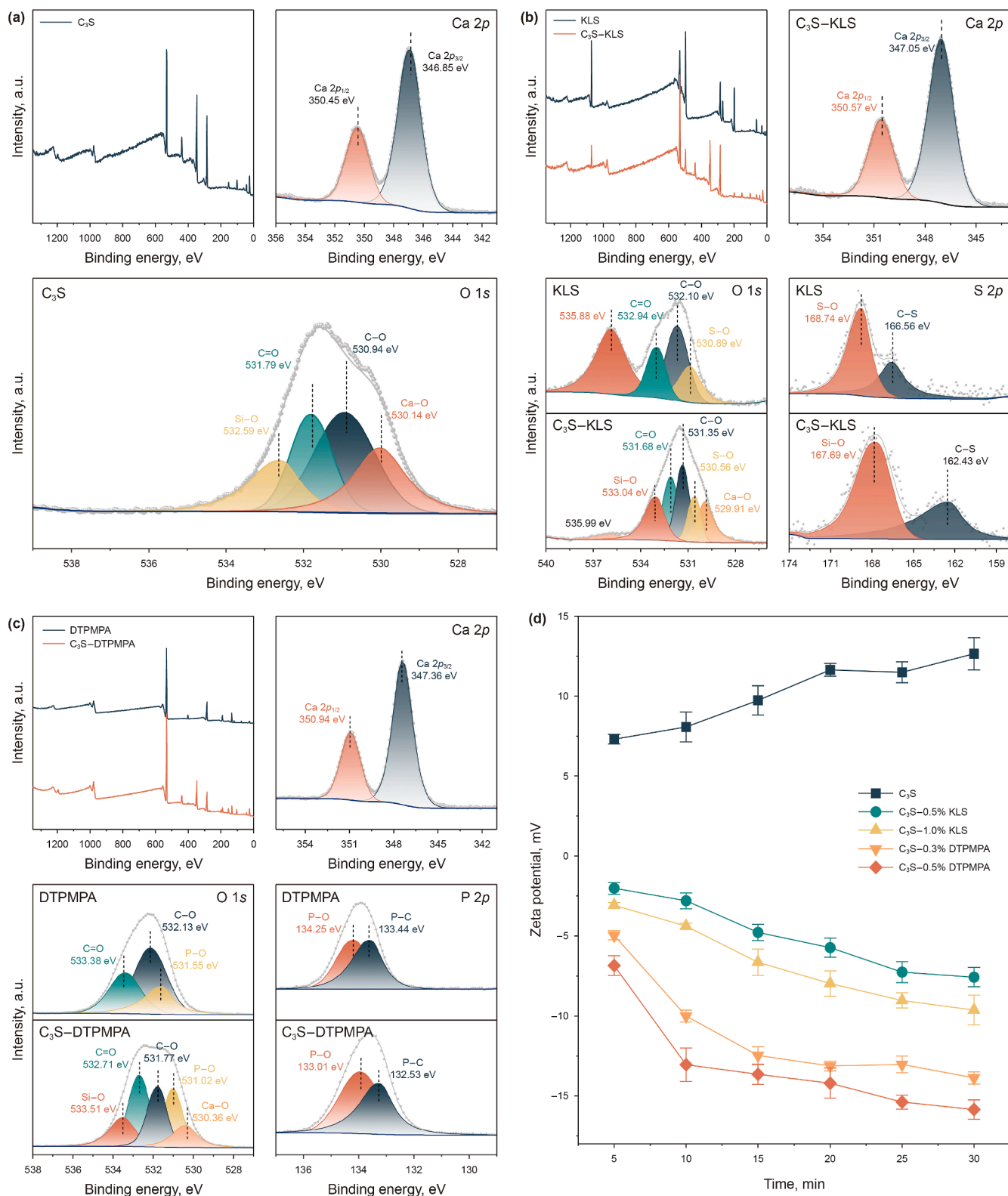


Fig. 5. (a) XPS spectrum of C_3S ; (b) XPS spectra of KLS before and after adsorption on C_3S ; (c) XPS spectra of DTPMPA before and after adsorption on C_3S ; (d) zeta potential variations of KLS and DTPMPA at different dosages over time.

being a small-molecule compound and having stronger functional groups for adsorption.

Cement clinker C_3S was used to investigate the interaction between the polymer KLS and the masking agent DTPMPA. After

stirring C_3S in water for 10 min, the mixture was filtered and freeze-dried (Fig. S6(a)). Upon adding a KLS solution to the C_3S suspension, followed by stirring and washing, a significant amount of polymer phase remained on the C_3S surface, located between

Table 2
Composition of the solution model.

Adsorption system	Analyzed spectral line	Original binding energy, eV	Binding energy after adsorption, eV	Charge transfer amount, eV
C ₃ S–KLS	O 1s (S–O)	530.89	530.56	–0.33
	S 2p (S–O)	168.74	167.69	–1.05
	Ca 2p _{3/2}	346.85	347.05	+0.20
	Ca 2p _{1/2}	350.45	350.57	+0.12
C ₃ S–DTPMPA	O 1s (P–O)	531.55	531.02	–0.53
	P 2p (P–O)	134.25	133.01	–1.24
	Ca 2p _{3/2}	346.85	347.36	+0.51
	Ca 2p _{1/2}	350.45	350.94	+0.49

the particles (Fig. S6(b)). EDS analysis of C₃S revealed a notable increase in the mass percentage of C, along with 3.16% S, after KLS adsorption (Fig. S6(e)). To evaluate the masking effect, DTPMPA was added to the C₃S solution and stirred for 15 min, followed by the addition of an equal mass of KLS and continued stirring for another 15 min. The solution was then washed and freeze-dried. It was observed that no polymer formed on the surface of C₃S (Fig. S6(c)). These results demonstrate that DTPMPA effectively masks the active sites on the C₃S surface, thereby inhibiting the subsequent adsorption of KLS particles.

3.2.2. Adsorption behavior of polymers and masking agents in metal ion solutions

To further investigate the adsorption strength of masking agents and polymer molecules on metal ions in cement filtrate, qualitative and quantitative analyses of metal ions were conducted using ICP (Caruso et al., 2017). Similar decreasing trends were observed in the concentrations of Al³⁺ and Fe³⁺ (Fig. 6(a, b)). As shown in Fig. 6(c), the test data indicated that the addition of KLS reduced the metal ion concentration. The concentration of Ca²⁺ decreased from 422.7 to 162.6 mg/L, whereas in the DTPMPA group, the residual Ca²⁺ decreased to 45.9 mg/L, indicating a significantly higher adsorption capacity than KLS.

Different amounts of masking agent (DTPMPA) were added to gel structures to analyze their efficacy in disrupting the cross-linked networks formed by other metal ions. The addition of 0.5% DTPMPA effectively disintegrated the gel structures formed by Al³⁺ and Fe³⁺ (Fig. 6(d–f)).

To simulate the high alkalinity and thermal conditions of cementing environments, the masking agent was added to the gel structures at pH 13 (Fig. 6(h)) and 90 °C (Fig. 6(i)). When 0.5% of the masking agent was added to the gel structure at pH 13, the gel structure formed by Al³⁺ almost completely disappeared, while the gel structure formed by Fe³⁺ decreased and turned into a reddish-brown homogeneous liquid (Fig. 6(h)). After being placed in a 90 °C water bath, the gel structure formed by Al³⁺ turned into a white homogeneous liquid. In contrast, the gel structure formed by Fe³⁺ dissolved, and the solution turned yellow (Fig. 6(i)). These findings demonstrate that an adequate dosage of the masking agent can effectively disintegrate gel structures, even under strong alkaline and high-temperature conditions.

3.2.3. Charge density and orbital information

From a computational perspective, this study analyzes the interactions among the small-molecule masking agent DTPMPA, the polymer KLS, and the cement slurry. First, molecular structure analyses of DTPMPA and KLS were conducted. Given the highly alkaline environment of cement slurry, the polar functional groups in these molecules undergo deprotonation. Therefore, in the simulations, the molecules were partially deprotonated, and their electrostatic potential (ESP) distributions were examined (Fig. 7(a, b)). In DTPMPA, the deprotonated phosphonate groups carried

significantly more negative charge than the deprotonated sulfonate groups (Zhang et al., 2021b).

The electron-donor and acceptor capabilities at different molecular sites were analyzed using frontier molecular orbitals. For the KLS polymer fragment, the E_{HOMO} and E_{LUMO} were determined to be –1.478 and 1.384 eV, respectively. In contrast, the DTPMPA exhibited a significantly higher E_{HOMO} (2.300 eV), suggesting its superior electron-donating capability compared to KLS (Fig. 7(c)). Meanwhile, DTPMPA exhibited a smaller band gap of only 1.709 eV, indicating higher molecular polarizability and enhanced chemical reactivity due to facilitated electron transitions. This characteristic may facilitate charge transfer with adsorbates, thereby enhancing its overall adsorption capacity.

3.2.4. Adsorption configurations and energy

To demonstrate the adsorption strength of KLS and DTPMPA on C₃S surfaces, charge density analysis was performed for both substances adsorbed on C₃S. As shown in Fig. 8(a, b), significant electron density overlap was observed between the two oxygen atoms of the phosphonate groups in DTPMPA and the calcium atoms on the C₃S clinker surface (Ding et al., 2023). Further computational analysis of adsorption configurations (Fig. 8(c)) revealed that two O atoms from the DTPMPA phosphonate groups formed bonds with Ca atoms on C₃S at distances of 2.322 and 2.424 Å. These distances are comparable to or shorter than the sum of the Ca–O ionic radii (2.43 Å), indicating bidentate coordination (Orazi et al., 2020). In contrast, although the sulfonate group in KLS can also form bonds with Ca atoms on the C₃S surface through a single oxygen atom (with a Ca–O bond length of 2.435 Å, slightly exceeding the sum of their ionic radii), bond length analysis reveals that the phosphonate groups in DTPMPA maintain closer distances to Ca atoms (Fig. 8(d)). Furthermore, the formation of both bridging and bidentate coordination modes in DTPMPA results in more stable bonding configurations.

Adsorption energy calculations were performed to further quantitatively compare the binding capabilities of KLS and DTPMPA on C₃S surfaces. The adsorption energy was calculated using Eq. (1):

$$E_{\text{ads}} = E_{(\text{ad}+\text{sub})} - E_{\text{ad}} - E_{\text{sub}} \quad (1)$$

where E_{ads} represents the adsorption energy of the molecule on the C₃S surface; E_{ad} is the self-energy of the molecule; E_{sub} denotes the intrinsic energy of the C₃S crystal; and $E_{(\text{ad}+\text{sub})}$ corresponds to the total energy of the system after molecular adsorption on the C₃S surface (Mishra et al., 2013a; Qi et al., 2021). The calculated adsorption energy results are presented in Table 3.

Based on the adsorption energy calculations, the study found that the adsorption energy of the small-molecule DTPMPA on the C₃S surface was –766.30 kJ/mol. In comparison, the adsorption energy of KLS polymer fragments was –365.77 kJ/mol, which is only half that of the DTPMPA system.

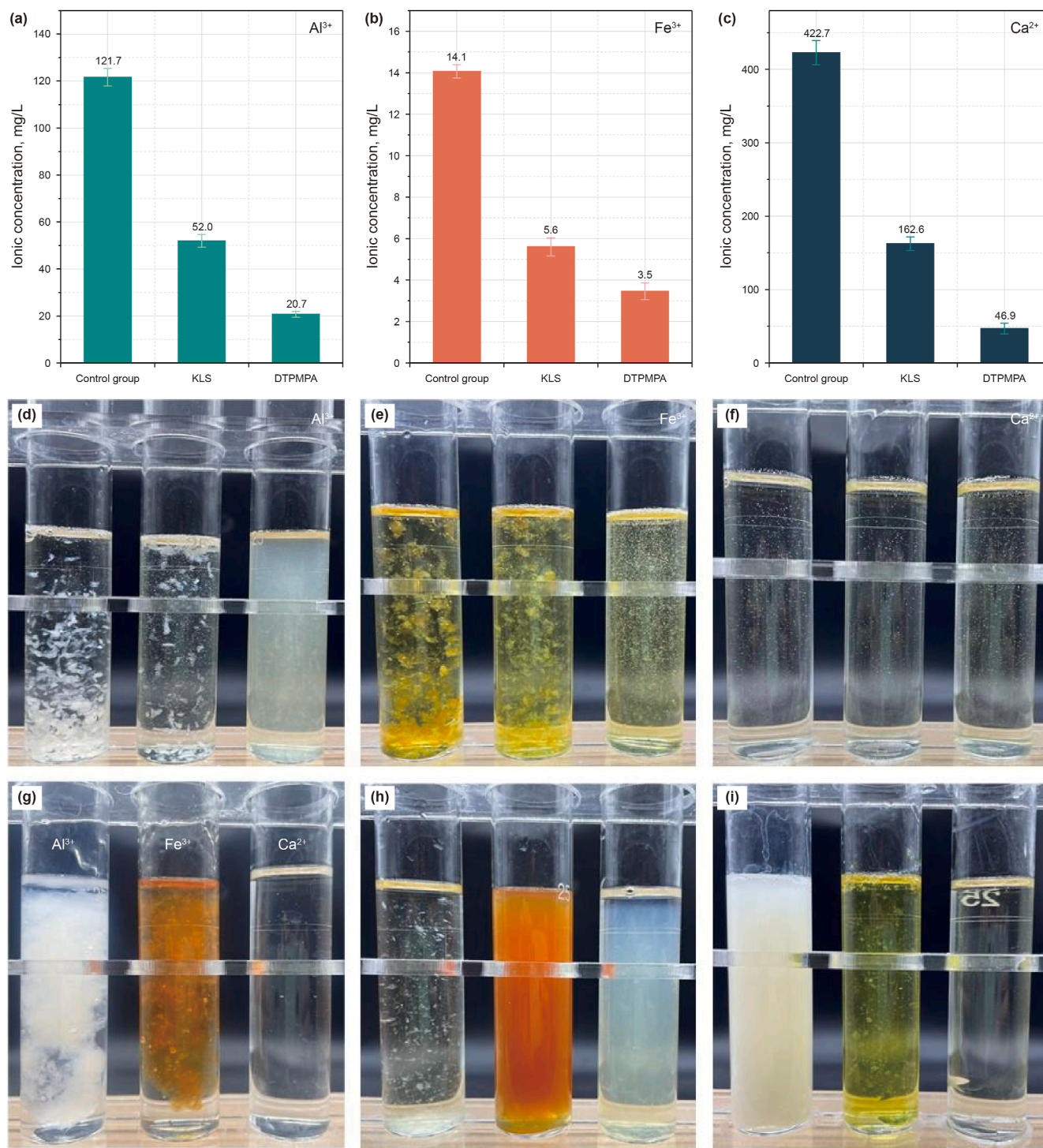


Fig. 6. Residual concentrations of metal ions in cement slurry filtrate: (a) Al^{3+} , (b) Fe^{3+} , (c) Ca^{2+} . Reactions between polymer KLS–metal ion complexes and masking agent under varying conditions (room temperature, pH = 7): addition of masking agents at 0.1%, 0.3%, and 0.5% (from left to right) to polymer KLS–metal ion complexes: (d) Al^{3+} , (e) Fe^{3+} , (f) Ca^{2+} . Chelation complexes between metal ions (Al^{3+} , Fe^{3+} , Ca^{2+} (from left to right)) and KLS under different conditions: (g) room temperature, pH = 7, without masking agent, (h) room temperature, pH = 13, 0.5% masking agent, (i), 90 °C, pH = 7, 0.5% masking agent.

To investigate the electronic behavior during the adsorption of sulfonate groups from KLS and phosphonate anions from DTPMPA on the C_3S surface, the projected density of states (PDOS) before and after adsorption (Wang et al., 2024). As shown in Fig. 8(f, g), the p orbital shift of Ca atoms on the C_3S surface after DTPMPA

adsorption exceeds that observed with KLS adsorption. For both the sulfonate group of KLS and the phosphonate group of DTPMPA, the oxygen orbital electrons are mainly occupied by the $2p$ and $2s$ orbitals. Following adsorption, the density of states (DOS) of surface O $2p$ orbitals decreased significantly near the Fermi level. It

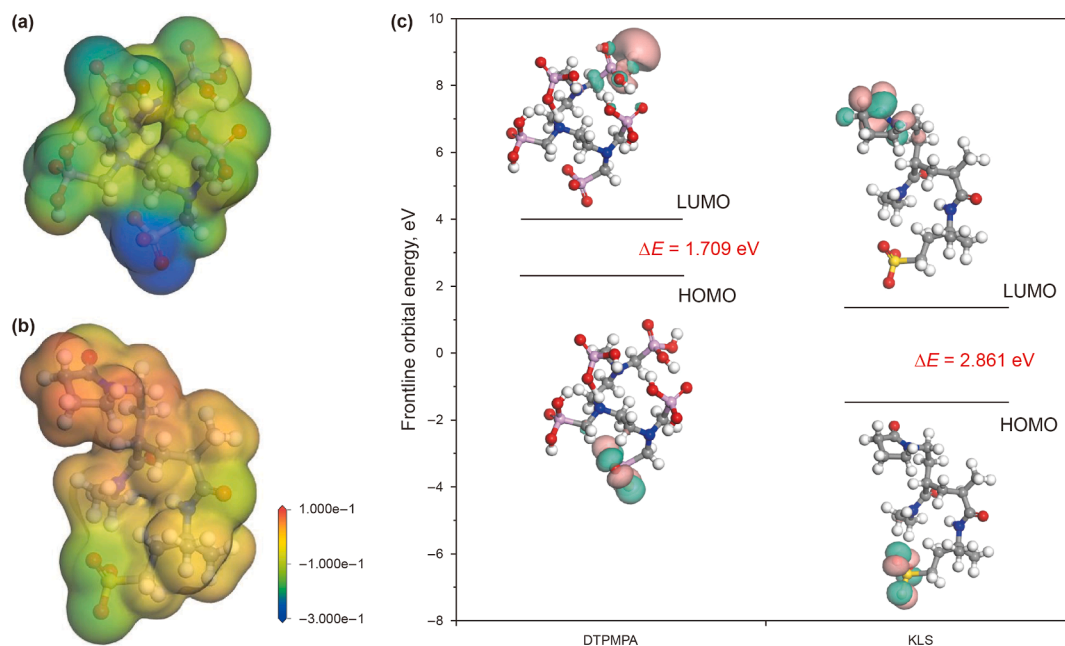


Fig. 7. Electrostatic potentials of DTPMPA (a) and KLS (b), and their frontier orbitals (c).

shifted toward the valence band, indicating electron donation from 2p orbitals to Ca atoms. In comparison, the displacement of the 2p valence band of the oxygen atom in the phosphonic group of DTPMPA (1.59 eV) is much greater than that of the oxygen atom in the sulfonic group of KLS (0.62 eV). Moreover, after adsorption, the DOS analysis revealed a significant orbital overlap between the p orbital of Ca and the s orbital of O at -20 eV, leading to Ca–O coordination and the formation of a chemical bond that enhances interfacial interaction (Fig. 8(h, i)). By comparing the interactions of KLS and DTPMPA with the surface Ca of C_3S_2 , it is found that the 2s orbital of oxygen in the phosphonic group of DTPMPA shifts and overlaps with the p orbital of Ca on the C_3S_2 surface, with the intensity of the overlapping peak being greater (Yang et al., 2024b).

3.2.5. Interatomic interaction

The radial distribution function is commonly used to show the strength of interactions between different substances. In this study, it is primarily used to assess the strength of interactions between the strong adsorption groups, sulfonic and phosphonic groups, in KLS and DTPMPA molecules with metal ions (Ca^{2+} , Al^{3+} , and Fe^{3+}) in cement slurry filtrate. First, the KLS analysis was conducted. As shown in Fig. 9(a), after KLS was added to the metal ion solution and molecular dynamics calculations were performed, the simulation results indicate that the sulfonic group in KLS interacts more strongly with Fe^{3+} than with Ca^{2+} or Al^{3+} . Furthermore, when both KLS and DTPMPA are simultaneously added to the metal ion solution, it was found that the interaction ability of the sulfonic group in KLS with metal ions was significantly reduced, with the strongest peak for Fe^{3+} only reaching 2.8 (Fig. 9(b)). By studying the interaction between DTPMPA and metal ions, it was found that when DTPMPA was added alone to the metal ion solution, the peak intensities of the phosphonic group in DTPMPA for Ca^{2+} , Al^{3+} , and Fe^{3+} were higher than those in KLS, with values of 30, 29, and 43, respectively (Fig. 9(c)). When both KLS and DTPMPA were simultaneously added to the metal ion solution, calculations showed that the interaction strength of the phosphonic group in DTPMPA with metal ions remained almost

unchanged. This demonstrates that DTPMPA has superior binding affinity for metal ions and effectively outcompetes KLS for them in solution (Fig. 9(d)).

3.3. Mechanism analyses

First, it was clarified that the leading cause of contamination is the large molecular polymers in the drilling mud treatment agents, which contain numerous strong adsorptive groups, such as carboxyl ($-COOH$) and sulfonic acid ($-SO_3H$) groups. Under the highly alkaline conditions of the cement slurry, these strong adsorptive groups deprotonate, leading to strong adsorption. Simultaneously, the hydration process of the cement slurry system generates numerous metal ions, and the cement particles' surfaces exhibit multiple active sites. When the cement slurry was mixed with the mud, the active, strongly adsorptive groups in the mud's polymer components interact with the metal ions and cement particles, leading to adsorption reactions between ions and particles. A gel-like network is formed, ultimately leading to contamination.

The design concept, based on the contamination mechanism, involves introducing a phosphonic acid-based masking agent with stronger adsorption properties into the cement slurry. This masking agent can occupy the active sites of metal ions and cement particles, thereby inhibiting the adsorption of potent polymer treatment agents in the slurry onto the cement, preventing gel structure aggregation. At the same time, the masking agent must meet the condition of adsorbing only to individual cement particles or metal ions, without cross-linking itself. Phosphonic acid-based small molecules with these characteristics can form multi-dentate coordination with cement particles or metal ions (Fig. 10). Through experiments and simulation calculations, it is found that the masking agent also exhibits competitive adsorption. Even if the polymer treatment agent forms cross-linked structures with metal ions or cement particles after adsorption, the masking agent can break down the structure and achieve the goal of decontamination.

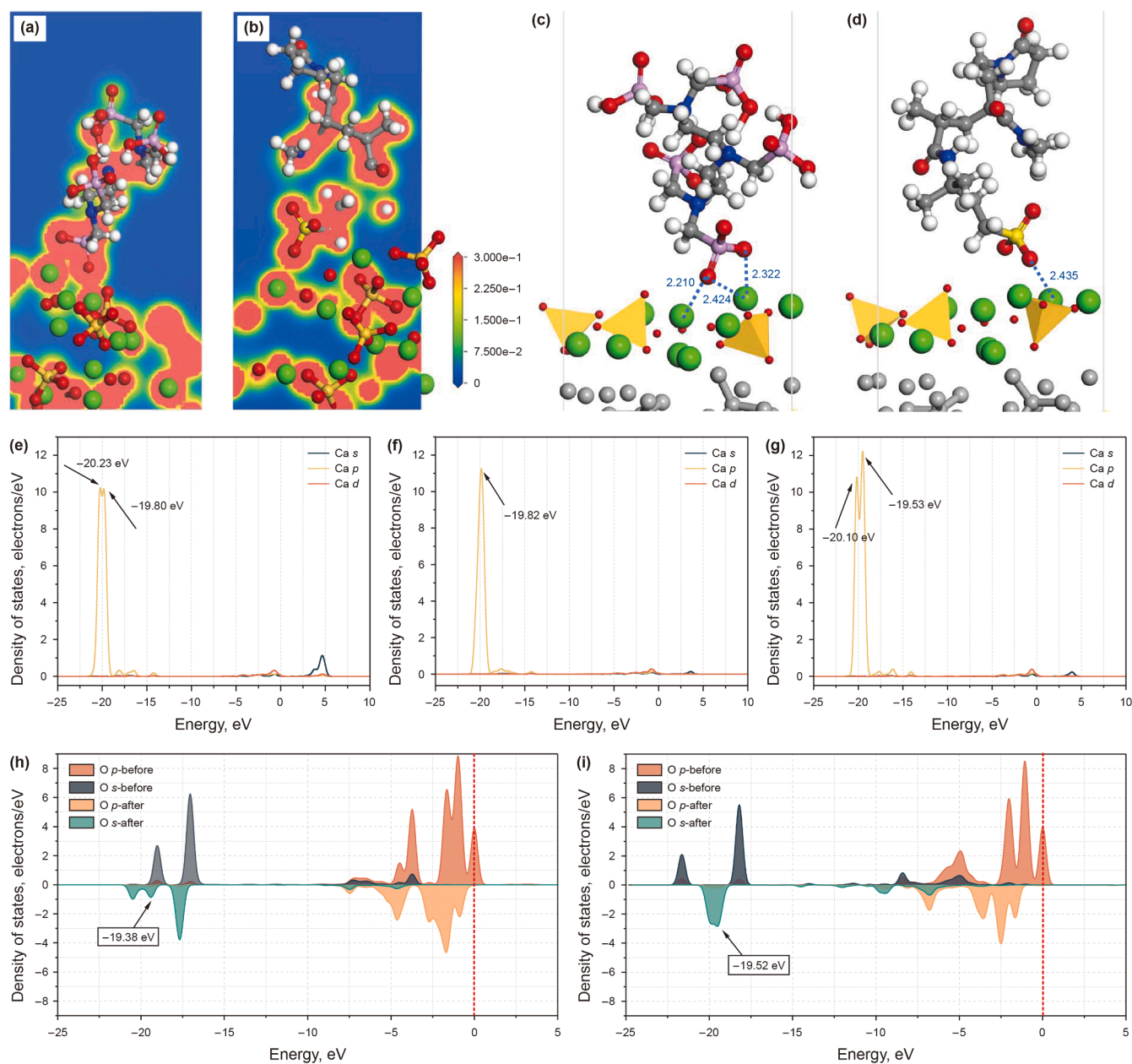


Fig. 8. Molecular surface charge density distributions of DTPMPA (a) and KLS (b); adsorption site of DTPMPA (c) and KLS (d) on C₃S surfaces; density of states (DOS) of Ca atoms on the C₃S surface before (e) and after adsorption of KLS (f) and DTPMPA (g); DOS of O atoms in the functional groups of KLS (h) and DTPMPA (i) before and after adsorption.

Table 3

Adsorption energy differences between DTPMPA and KLS on the C₃S surface.

$E_{\text{ads}}(\text{DTPMPA})$, kJ/mol	$E_{(\text{ad} + \text{sub})}(\text{DTPMPA} + \text{C}_3\text{S})$, kJ/mol	$E_{\text{ad}}(\text{DTPMPA})$, kJ/mol	$E_{\text{sub}}(\text{C}_3\text{S})$, kJ/mol
-766.30	-51318196.62	-8813329.79	-42504100.52
$E_{\text{ads}}(\text{KLS})$, kJ/mol	$E_{(\text{ad} + \text{sub})}(\text{KLS} + \text{C}_3\text{S})$, kJ/mol	$E_{\text{ad}}(\text{KLS})$, kJ/mol	$E_{\text{sub}}(\text{C}_3\text{S})$, kJ/mol
-365.77	-47117994.94	-4613466.79	-42504162.38

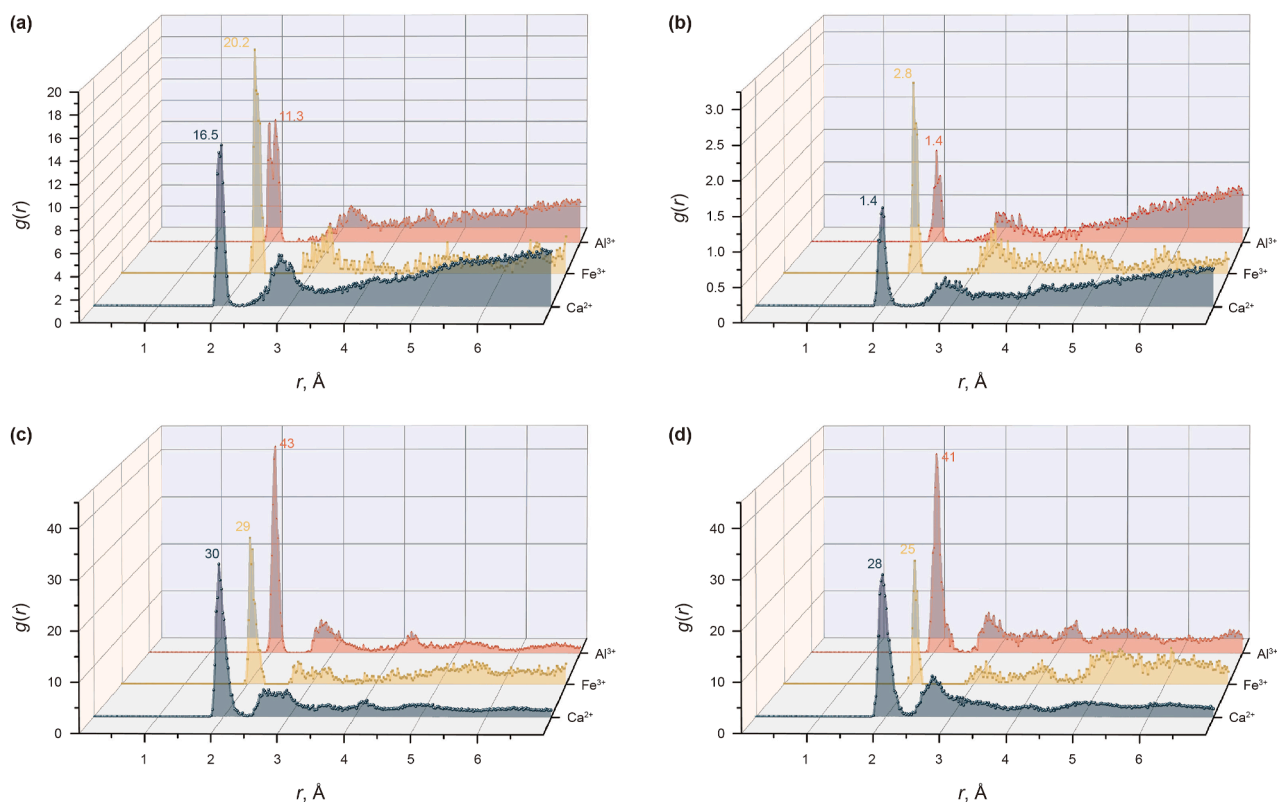


Fig. 9. Radial distribution function of molecules and metal ions. (a) KLS and metal ions; (b) KLS and metal ions in the mixed solution of KLS and DTPMPA; (c) DTPMPA and metal ions; (d) DTPMPA and metal ions in the mixed solution of KLS and DTPMPA.

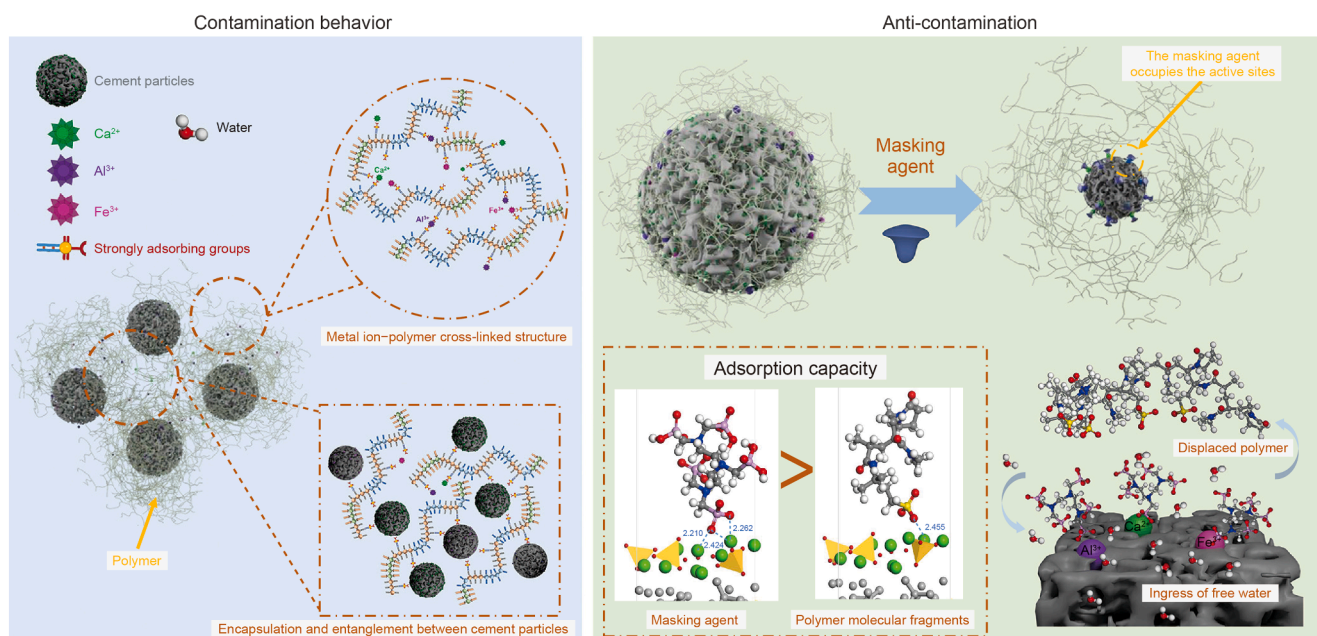


Fig. 10. Mechanism diagram.

3.4. Effect of the masking agent on contamination inhibition

3.4.1. Effect of masking agents on the performance of contaminated cement slurry

To assess the anti-contamination efficacy of the masking agent in OWC, the agent was added to OWC at a mixing ratio of 7:3 (OWC:WBM) for a contamination test. After adding the masking agent, the thickening performance of the contaminated OWC was significantly improved. With the addition of 0.3% masking agent (Fig. 11(a)), the thickening times for the 7:3 mixing ratio were extended from 94 to 220 min. When the addition was increased to 0.5%, the thickening time met the required specifications, and the contaminated slurry thickening curve became stable (Fig. 11(b)).

To further investigate the improvement of the masking agent on the flowability and compressive strength of the 7:3 mixed contaminated cement slurry, 0.3% and 0.5% of the masking agent were added for compressive strength and flowability testing. Under the 7:3 mixing ratio, after adding 0.3% masking agent, the compressive strength increased from 0 to 7.2 MPa after 2 d. With the addition of 0.5% masking agent, the compressive strength improved by 158% after 7 d (Fig. 11(c)). After curing at 90 °C, the flowability of the contaminated slurry with 0.3% masking agent increased from 8.7 to 17.7 cm, and further increased to 23.7 cm with the addition of 0.5% masking agent (Fig. 11(d)) (Zhang et al., 2024b). Considering that related studies have shown that the addition of the masking agent can affect the hydration degree of cement slurry, we investigated the changes in the thickening time of the cement slurry after adding 0.3% and 0.5% of the masking agent. The thickening experiment found that with a 0.3% addition, the thickening time was extended by 75 min; with a 0.5% addition, the thickening time was extended by 100 min, indicating that the masking agent has a certain effect on the extension of the thickening time of the cement slurry (Fig. 11(e, f)). The mechanism for the extended thickening time may be that the phosphonic acid groups in the masking agent occupy the CSH nucleation sites on the surface of C_3S , thereby reducing the nucleation rate and number of CSH, which delays the hydration process of C_3S and

leads to the formation of hydration products such as CSH gel and CH. At the same time, the complexation of the masking agent with Ca^{2+} in the solution further prolongs the induction period by preventing CSH from reaching the supersaturation required for precipitation. Ultimately, this results in a slight delay effect in the cement slurry (Huang et al., 2022; Kupwade-Patil et al., 2019; Zou et al., 2024).

The effect of the masking agent on the compressive strength of the cement slurry was also studied. As shown in Fig. 11(g), the experimental results indicated that on the first day of curing, as the addition of the masking agent increased, the compressive strength decreased. After 7 d of curing, the decrease was less than 17%. After 14 d of curing, the masking agent had no effect on the strength development of the set cement.

To compare with the anti-contamination effect of the masking agent, 0.5% citric acid was added to the cement slurry as a control group. The thickening test of the cement slurry mixed with WBM (7:3) is shown in the thickening curve in Fig. S7(a). The thickening time was 268 min, significantly shorter than that of the cement slurry, resulting in abnormal gelation. After the experiment, it was found that the internal portion of the sample removed was not completely solidified, as shown in Fig. S7(c). Furthermore, spacer fluid was used to mitigate the contamination of the cement slurry by WBM. A thickening test was conducted on a contaminated mixture of cement slurry, spacer fluid, and WBM at a mixing ratio of 7:1:2, as shown in Fig. S7(b). The thickening time was 273 min, which was still less than that of the cement slurry.

To verify the adaptability of the masking agent under high-temperature, high-pressure, and high-salinity conditions, cement slurry formulations and WBM used in the field application at the GT well in Xinjiang were selected. The anti-salt cement slurry formulations are shown in Tables S5 and S6, with conditions set at 164 °C, 123 MPa, and 70 min. The thickening test of the cement slurry is illustrated in Fig. S8(a), with a thickening time of 400 min. When the cement slurry was mixed with a sulfonated water-based drilling fluid in a 7:3 ratio, the initial consistency exceeded 30 Bc, and an abnormal thickening phenomenon occurred at 120 °C,

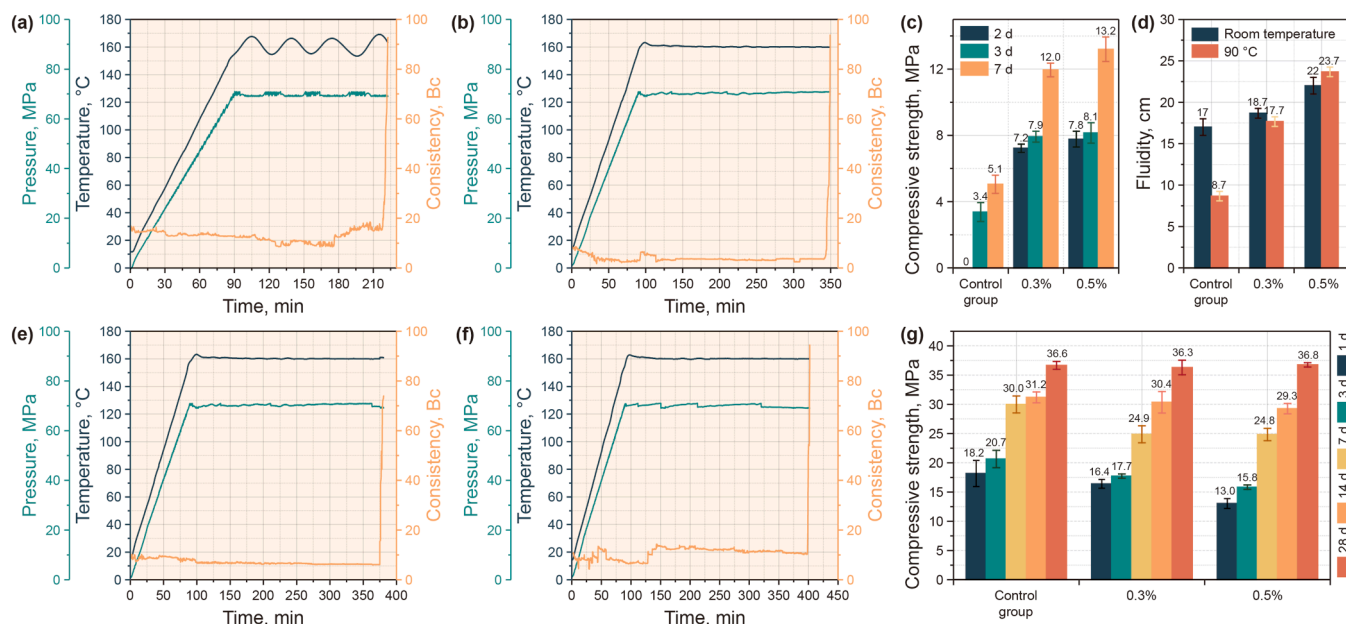


Fig. 11. Contamination resistance tests with different masking agent dosages, OWC at a mixing ratio of 7:3 (OWC:WBM): (a) 0.3% dosage thickening test, (b) 0.5% dosage thickening test, (c) compressive strength, (d) flowability. Effect of different dosages of the masking agent on the performance of cement slurry: (e) thickening experiment with a 0.3% dosage, (f) thickening experiment with a 0.5% dosage, (g) compressive strength at different curing periods.

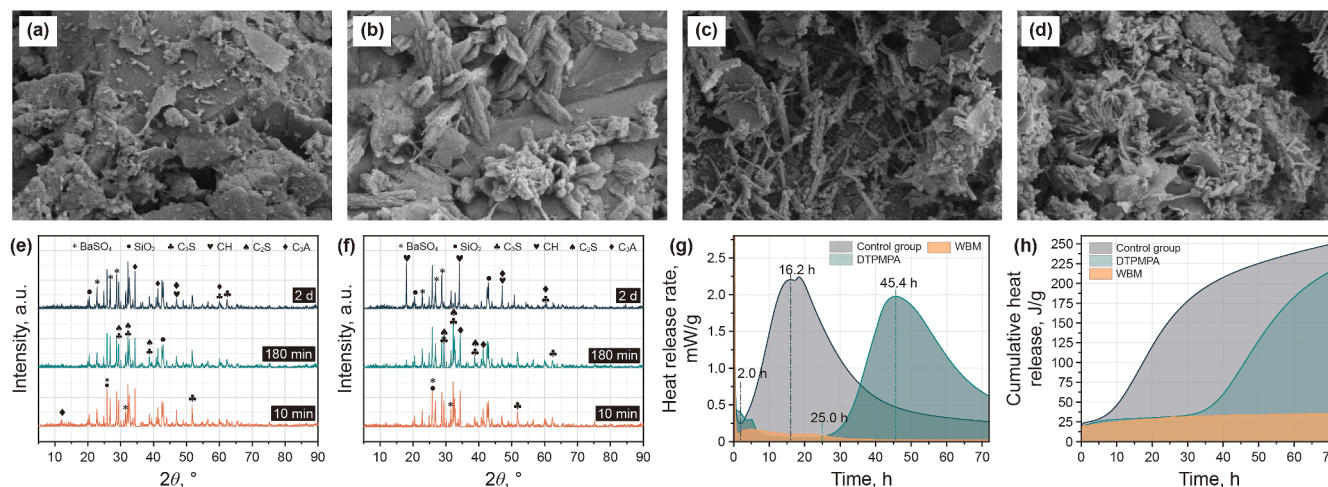


Fig. 12. Analyses of contaminated cement slurry without (a, b, e) and with (c, d, f) treated with masking agent. Control group: (a) SEM image after 180 min of hydration; (b) SEM image after 2 d of hydration; (e) XRD phase analysis. Masking agent-added group: (a) SEM image after 180 min of hydration; (b) SEM image after 2 d of hydration; (e) XRD phase analysis. Heat release rate (g) and cumulative heat release (h) of the cement slurry (control group), cement slurry containing WBM and contaminated cement paste containing DTPMPA.

shortening the thickening time to 68 min (Fig. S8(b)). After adding 0.5% of masking agent to the cement slurry, the thickening time of the slurry mixed in a 7:3 ratio extended to 450 min, and the slurry remained stable, as shown in Fig. S8(c). Furthermore, the impact of the masking agent on the compressive strength of the set cement was analyzed, as illustrated in Fig. S8(d). After the addition of the masking agent, there was a certain effect on strength development; after 3 d of hydration, the compressive strength decreased by 16%, while mixing in a 7:3 ratio increased the compressive strength by 12%. The addition of the masking agent effectively improved the compatibility between the cement slurry and the drilling fluid.

3.4.2. Effect of masking agents on the microstructure and hydration of contaminated cement slurry

SEM analysis was conducted on WBM contaminated cement slurry at different hydration times. Without the addition of the masking agent, at 180 min of hydration time, a film-like substance appeared on the surface of the cement particles (Fig. 12(a)). After 2 d of curing, the surface of the cement paste showed almost no hydration products (Fig. 12(b)). In contrast, with the addition of the masking agent, at 180 min of hydration (Fig. 12(c)), the surfaces of the cement particles remained uncovered, while CH and Aft were produced, and a large number of particles were embedded on the clinker surfaces, which might be residual inert substances from the WBM. After 2 d of hydration time (Fig. 12(d)), a significant amount of needle-like CSH hydration products appeared. Further XRD analysis investigates the effect of contaminated cement slurry and the addition of a masking agent on cement hydration products. It can be observed that, due to the complexity of the WBM, the diffraction patterns are relatively complex, allowing detection of phases such as barite (BaSO_4) and quartz sand (SiO_2). It was observed that the addition of WBM significantly reduced the degree of cement hydration, with the characteristic peaks of C_3S , C_3A , and C_2S still present after 2 d of hydration, while the characteristic peaks of cement hydration products CH was of lower intensity (Fig. 12(e)). As shown in Fig. 12(f), when the contaminated cement slurry was treated with the masking agent, there are significant changes in both the cement clinker and hydration products. At 180 min of hydration, the characteristic CH peak appeared in the sample. As hydration continues for 2 d, the characteristic CH peak

strengthens. Analysis of the relative content of crystal phases revealed that, after the addition of DTPMPA, the proportion of CH increased from 1.2% to 21.2% (Fig. S9). The original curve and the fitting residuals are shown in Fig. S10. At the same time, the characteristic peak of C_3A was significantly weakened, and the most notable change was the almost complete disappearance of the characteristic peaks of C_3S and C_2S .

To investigate the impact of WBM contamination and the addition of a masking agent on heat release during cement hydration, isothermal calorimetry was used to measure heat release over the first 72 h of hydration. It is pertinent to note that data from the initial 60 min may not accurately reflect the true heat release because the sample requires time to attain a stable heat flow within the calorimeter. As shown in Fig. 12(g), the heat release rate curve for the control group comprises an induction period, an acceleration period, and a deceleration period. However, compared to the 252 J/g heat release of the control group cement slurry, the cement slurry containing WBM showed no significant heat release during the acceleration period after the induction period. The cumulative heat release after 72 h was only 36 J/g, a decrease of 86% (Fig. 12(h)). Adding a 0.5% masking agent effectively mitigated hydration of the contaminated cement slurry. Compared to the control group, the induction period was extended to 25 h, resulting in an extended acceleration period of 45.4 h. However, the cumulative heat release at 72 h showed only a 12% decrease compared to the control group, indicating a significant enhancement in the hydration of the contaminated cement slurry.

4. Conclusions

Based on the above findings, this study provides a detailed explanation of the mechanism by which DTPMPA mitigates contamination from WBM. Initially, single-factor analysis identified that strongly adsorbing macromolecular additives in the WBM as the fundamental cause of OWC performance degradation. Experiments and simulation calculations confirmed that the phosphonic acid molecule (DTPMPA), as a masking agent, can effectively isolate the interference from drilling fluid additives on cement slurry.

The addition of the masking agent to the cement slurry significantly improved performance parameters, including

thickening time, fluidity, and compressive strength. Additionally, evaluations confirmed that the masking agent had minimal impact on both the compressive strength and thickening time of the cement slurry.

In conclusion, this study identifies macromolecular polymers in WBM as the primary cause of cement slurry contamination and fully elucidates the protective mechanism of the masking agent. Given its stronger chemical adsorption on cement mineral surfaces, DTPMPA has significant potential for use in high-temperature deep and ultra-deep wells, where reinforced chemical bonds are better able to resist desorption at high temperatures. In practical applications, the masking agent must work synergistically with other additives, such as dispersants, retarders, and fluid-loss agents. Therefore, investigating the compatibility of DTPMPA with common OWC additives remains a crucial area for future research.

Future work should focus on the performance evaluation of cement slurry systems that closely simulate downhole conditions and on their adaptability across different geological environments.

CRediT authorship contribution statement

Yuan Gao: Writing – original draft, Resources, Methodology, Conceptualization. **Lei Yang:** Writing – review & editing, Validation, Resources, Data curation. **Sheng Huang:** Writing – review & editing, Supervision, Project administration, Methodology, Funding acquisition, Conceptualization. **Tao Zhen:** Validation, Resources, Investigation, Formal analysis. **Miao Xu:** Resources, Methodology, Investigation. **Zao-Yuan Li:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization. **Zi-Yan Ren:** Visualization, Formal analysis, Data curation. **Xin-Zhe Zhou:** Validation, Methodology, Formal analysis. **Hai-Bo Cheng:** Visualization, Validation, Formal analysis. **Xing-Yu Peng:** Visualization, Validation. **An-Ming Liao:** Visualization, Validation.

Declaration of competing interests

The authors 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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Supplementary data

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