Impact of aluminium acetate particles size on the gelation kinetics of polyacrylamide-based gels: Rheological and molecular simulation study

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Abstract
Inorganically crosslinked polymers have been intensively implemented for conformance control treatments in oil and gas wells at low temperatures (<90°C) because of their faster gelation time compared to organically crosslinked gels. Crosslinkers such as chromium acetate are known to be toxic, and aluminium-based alternatives have been introduced. This study aims to investigate the impact of aluminium acetate (AlAc) particle size on the gelation kinetics of polyacrylamide (PAM)-based gels at a pH of 5 and temperature of 75°C. Moreover, bentonite is used as an additive to delay the crosslinking of PAM/AlAc gels. Reducing the particle size increases the specific surface area of the particles and provides more crosslinking sites. Therefore, lower PAM concentrations (up to 5 wt.%) could be used without AlAc settling. Using 7 wt. % PAM/1 wt.% AlAc with sizes of 25 and 48 μm revealed a crosslinking time of 17 and 115 min, respectively. The addition of bentonite at low crosslinker concentrations (0.5–1 wt.%) did not decrease the gel strength of 7 wt.% PAM/1 wt. % AlAc significantly. The gelation time was extended after adding 1 wt.% bentonite to the formulation where the delay was attributed to the adsorption of AlAc on the bentonite surface that was illustrated by molecular simulation.

KEYWORDS
aluminium acetate, conformance control, crosslinking, gelation, polyacrylamide

1 INTRODUCTION

Lost circulation is one of the major difficulties during the drilling of oil and gas wells in which the drilling fluids are accidentally lost in the fractured formations after using high mud density. Lost circulation considerably increases the cost of drilling operations because of the extension of the non-productive time and further treatment of the fractured zone. The shrinkage of the mud weight window (MWW) is a challenge during drilling high pressure and high temperature (HPHT) wells, fractured formations, and depleted reservoirs. Recently,
polymeric formulations have been introduced as lost circulation materials (LCMs) for wellbore strengthening to overcome the limitations of conventional LCMs, such as high concentrations and large particle sizes.\textsuperscript{[1,2]} Plugging the fractures near the wellbore prevents further mud losses while extending the MWW, which facilitates drilling in abnormal formations.\textsuperscript{[3]}

Polyacrylamide (PAM)-based formulations crosslinked with organic and inorganic crosslinkers have been widely implemented in conformance control applications.\textsuperscript{[4]} Organic crosslinkers, such as polyethyleneimine (PEI), have provided high gel strength and revealed high thermal stability at high temperatures (>90°C).\textsuperscript{[5,6]} Furthermore, inorganic crosslinkers are preferred over organic crosslinkers at lower temperature range.\textsuperscript{[7]} Many types of inorganic crosslinkers have successfully developed a gel with PAM through a coordination bond, such as chromium (Cr\textsuperscript{3+}), aluminium (Al\textsuperscript{3+}), and cobalt (Co\textsuperscript{2+}).\textsuperscript{[8,9]} The acetate group was reported to have the best controllable gelation performance as well as retardation effect since inorganic crosslinkers are sensitive to pH and rapidly form a gel at low pH.\textsuperscript{[10]} Table 1 summarizes some of the studied crosslinkable polymeric systems in the literature. The crosslinking systems reported in Table 1 can be applied to both sandstone and carbonate reservoirs. However, minerals such as acid-sensitive minerals in carbonate reservoirs and clays in sandstone reservoirs might affect the crosslinking.

Aluminium-based crosslinkers have been implemented as an environmentally friendly alternative to toxic chromium acetate, which was commonly implemented for conformance control in the oil and gas fields.\textsuperscript{[10,15–17]} Aluminium citrate crosslinked PAM and revealed a potential for in-depth control treatments. Moreover, aluminium acetate (AlAc), aluminium nitrate, and aluminium amino acetate were able to crosslink 9 wt.% PAM at different pH levels. Aluminium nitrate/PAM gelation was rapid and uncontrollable at pH > 4 with limited control at pH of 3, while the gelation kinetics of aluminium amino acetate with PAM are controllable at the pH range 6–9. AlAc outperformed the other two types with controllable gelation at pH between 4–6. Adding nanosilica to AlAc and aluminium/PAM solutions extended their pH controllable range to 9 and 10, respectively. The solution of 9 wt.% PAM/3 wt.% AlAc revealed thermal stability up to 100°C with a gelation time of up to 80 min at 75°C in a pH-controlled environment, which makes it suitable for low-temperature reservoirs.\textsuperscript{[10]} Nevertheless, settling of the crosslinking particles was reported as the main limitation, as the settling rate in some conditions exceeds the gelation rate, leading to a lower crosslinking ratio and less final gel strength.

Bentonite is one of the most used conventional mud additives as it acts as a weighting material.\textsuperscript{[18]} The required amounts vary depending on the engineering limitations, such as the capability of the pump and the mud weight window. The effect of these additives has been investigated with the crosslinkable polymeric systems and showed good compatibility.\textsuperscript{[1]} Tessarolli et al.\textsuperscript{[19]} investigated the effect of bentonite on an organically crosslinked polymeric system with PEI. The study revealed that bentonite affected the thermal stability of the system positively by reducing the viscosity as well as increasing the gelation time without having a significant impact on gel strength. Zolfaghari et al.\textsuperscript{[20]} considered the influence of another clay, montmorillonite, on an inorganically crosslinked system with chromium acetate. The introduction of the clay particles to the system enhanced its strength, which gives the system the ability to be used for wellbore strengthening. Furthermore, Magzoub et al.\textsuperscript{[21]} have developed a PAM-based drilling fluid using PEI as a crosslinker. The study revealed that the polymer-based mud (PBM) has a higher initial viscosity in the ambient conditions compared with the conventional water-based mud. However, the viscosity becomes less of an issue at elevated temperature due to the high shear thinning exhibited by the PBM. The study recommended a concentration of PAM between 5–7.5 wt.% as a reasonable range to avoid pumpability issues. Therefore, bentonite will be investigated in this study to evaluate its effect on the stability of the formulation.

In our previous work,\textsuperscript{[10]} the effect of concentration, salinity, temperature, and pH was investigated in PAM/AlAc system. However, particles stability was reported as the main limitation in this system. Therefore, the effect of crushed (smaller size) crosslinker particles and bentonite additives are investigated in this paper with an aim to enhance the stability of the gelant. In this work, the impact of the size of AlAc particles on the gelation kinetics of PAM/AlAc formulations is investigated by both experimental and theoretical techniques. This study aims to reduce the size of AlAc particles to hinder particles settling, which was reported as a shortcoming in this system. Rheological characterization supported by particle size measurements is employed to study the effect of particle size and the addition of bentonite in PAM/AlAc gel development. Furthermore, the mechanism of bentonite interaction with the crosslinker is studied using the molecular simulation technique.

\section*{2 \quad EXPERIMENTAL WORK}

\subsection*{2.1 \quad Materials}

PAM polymer with a molecular weight of 700 000 Da was obtained from SNF Fogler, France. AlAc (purity of
99%) (Figure 1) was received from Glentham Life Sciences, England. One of the most common drilling fluid additives, bentonite, was added to the polymer/crosslinker-based solution to develop a polymer-based mud for wellbore strengthening applications.

2.2 | Size reduction of AlAc

A ball milling machine was used to crush the raw AlAc from an original size of ~65 μm to 48 μm and 25 μm. The milling process was accomplished in stages to avoid overheating the sample. The size of the AlAc particles was measured using a laser particle size analyzer (NANOTEC 22) manufactured by Frisch Company, Germany. The particle size measurements were done under wet dispersion in water.

2.3 | Polymer-based mud preparation

For the PAM/AlAc system, the polymer (PAM) was initially put in a beaker and diluted to the desired concentration, then AlAc was slowly added to the solution. The mixing time is 1 h, in the case of the 65 μm AlAc, to avoid settling of the particles, while for the smaller sizes the stirring time was kept up to 10 min. AlAc should be gradually added to avoid agglomeration and settling to produce stable formulations. On the other hand, bentonite was dispersed in deionized water, then the PAM followed by AlAc solutions were added, according to the pre-specified concentrations. Our previous study[10] showed that PAM/AlAc system is most stable at the pH range between 4–6; therefore, the pH of all investigated systems in this paper has been fixed at 5.

2.4 | Rheological characteristics

The viscoelastic properties of the developed gels were investigated using an Anton Paar MCR 302 rheometer. The storage modulus (G’) was measured to evaluate the gel strength of the developed gel samples after aging in an oil bath for 24 h. Frequency sweep tests (1–100 Hz) at a strain of 10% were conducted on parallel plate geometry that has a 25 mm diameter with a 2 mm gap. Frequency sweep experiments were performed in duplicate and an error of less than 5% was ensured. Moreover, the gelation profile of the optimized polymer-based mud formulation with the drilling additives was compared to the base solutions, 7 wt.% PAM/1.5 wt.% AlAc, and 7 wt.% PAM/1.5 wt.% AlAc/0.5 wt.% AlAmAc using high-pressure cell geometry (CC25) which was loaded on CPTD-200 at a frequency of 10 Hz, strain of 10%, and temperature of 75°C. The high-pressure cell was pressurized by pure nitrogen gas (N2) and all the measurements were conducted at 500 psi (3.45 x 10^6 Pa).[10] This pressure is enough to keep water in the liquid phase as per our previous literature reports, and the selected strain was in the linear viscoelastic range.

**TABLE 1** Comparison between some crosslinking systems

| System (base polymer/crosslinker) | Gelation time | Temperature application range | Limitations | Ref. |
|----------------------------------|---------------|-------------------------------|-------------|-----|
| PAM/PEI                          | 27–194 min    | 85–140°C                      | Does not suit the low-temperature reservoirs. | Al-Muntasheri et al.[11–13] |
| PAM/Cr^{3+}                      | 3–8 days      | 65–80°C                       | Relatively toxic compared to other crosslinkers. | El-Karsani et al.[4,14] |
| PAM/Co^{2+}                      | -             | 130°C                         | Does not crosslink at temperatures of less than 130°C. | Nimir et al.[9] |
| PAM/Al^{3+}                      | 50–80 min     | 25–100°C                      | Settling of the crosslinking particles as they are insoluble in water. | Shamlooh et al.[10] |

**FIGURE 1** Chemical structure of aluminium acetate (AlAc)
3 | RESULTS AND DISCUSSION

3.1 | AlAc size reduction

A ball milling machine was used to crush AlAc particles from an initial size of ~65 μm to about 25 μm in three stages to avoid overheating the sample. The size distribution of the particles was compared before and after milling using a particle size analyzer. The measurements revealed that the AlAc particles’ size dropped to an average size of 25 μm (Figure 2). The particle size analysis showed that the specific surface area of the AlAc particles increased from 2474 cm²/cm³ for the original particles (65 μm size) to 3280 and 11 585 cm²/cm³ after reducing the size to 48 and 25 μm, respectively. Figure 3 reveals the specific surface area of AlAc particles at different sizes.

3.2 | Effect of AlAc particles size on the gelation of PAM

AlAc with the size of 65 and 25 μm and concentration of 3 wt.% was used to crosslink 9 wt.% PAM at a temperature of 75°C and pH of 5. Initially, adding AlAc at a size of 65 μm to 9 wt.% requires mixing the solution for 1 h to have a homogeneous system. Nevertheless, the developed gel showed a phase separation (about 19%) because of the settling of the AlAc particles (Figure 4). On the other hand, reducing the size of AlAc particles to about 25 μm enhanced the gel stability at similar conditions and considerably decreased the phase separation in the developed gel to ~3%.

The improvement of the gel stability after using the 25 μm AlAc particles is attributed to the better distribution of the particles on PAM chains, and hence more crosslinkable sites are easily reached compared to the 65 μm particles. Furthermore, using 25 μm AlAc particles...
shortened the mixing time with PAM to about 10 min instead of 1 h in case of the 65 μm size. However, a gel was noticed at room temperature (25°C) after 10 min when 3 wt.% AlAc (25 μm) was mixed with 9 wt.% PAM, indicating the fast gelation after AlAc size reduction. AlAc particles at a size of 65 μm settle when a low concentration of polymer is used, which triggers phase separation because of the settling of the particles and extends the gelation time. In oil and gas field practice, the polymer concentration is vital for pumping the crosslinking system; high viscosity causes difficulties in pumping and might lead to fracturing the formation. Furthermore, high polymer concentration accelerates the gelation time, which would be improper in the case of in-depth conformance control treatments. One of the advantages of AlAc size reduction is the ability to crosslink PAM at a wide range of concentrations with controllable gelation time. Figure 5 illustrates the effect of varying PAM concentration on the gel strength after adding 3 wt.% of AlAc particles with a size of 25 μm.

The largest size of 65 μm AlAc provided a slightly higher gel strength than the other smaller sizes; however, the formed gel is not homogeneous. This could be a consequence of the settling because the gel at the bottom of the test tube had a higher storage modulus (2252 Pa) compared to the upper part, where a very weak flowing gel was produced.

Figure 6 reveals the ability of 25 μm AlAc to crosslink PAM at various concentrations ranging from 5–9 wt.%. This advantage is crucial in field application because it enables the engineers to adjust the formulation to the required viscosity, and the gel will form in a reasonable time. Using 65 μm AlAc to crosslink PAM at low concentrations, such as 5 and 7 wt.%, did not produce gels within 24 h of aging. This can be explained by the impact of the polymer concentration on the gelation time since the low polymer concentration results in a long gelation time.

The 7 wt.% PAM was chosen as an optimum concentration of the polymer because the viscosity of the formulation is acceptable for the conformance control treatment in the field. Moreover, decreasing the concentrations of the polymer and crosslinker provides an opportunity to add other additives to the formulation, such as stabilizers and strengthening agents. Figure 7 shows the impact of the 25 μm AlAc concentration on the gel strength after crosslinking 7 wt.% PAM. A wide range of the crosslinker was used (0.5–3 wt.%) to crosslink 7 wt.% PAM. Gels were obtained in all formulations even with low concentration of 0.5 wt.% AlAc. Reducing the concentration of AlAc decreased the gel strength to about 350 Pa for 7 wt.% PAM/0.5 wt.% AlAc, whereas no gel formed when 65 μm size was incorporated into the PAM/AlAc system at the same concentrations. The use of low concentrations of AlAc reduces the cost and environmental impact of the gelling system in comparison with typical concentrations of the toxic chromium (III) acetate (0.1–0.5 wt.%[22,23]).

3.3 Impact of bentonite on the gelation of PAM/AlAc system

Additives, commonly mixed to formulate drilling fluids such as bentonite, are generally used with crosslinked polymers for different purposes, such as gel strengthening and
Using low concentrations of the PAM/AlAc would facilitate mixing drilling fluids additives because the viscosity remains in an acceptable range for field applications.

Bentonite is the most common additive in drilling fluids. Many studies have revealed its usefulness as a retarder for organically crosslinked gels. However, only a few studies have investigated the impact of clays on the gelation kinetics of the inorganically crosslinked gels.\[20,25\] Firstly, the bentonite is dispersed in water at a high steering speed to avoid the flocculation of the particles. Then PAM was added gradually at the pre-specified concentration followed by AlAc. PAM is adsorbed on the bentonite surface via hydrogen bonding.\[26\] Bentonite could physically shield the crosslinking sites of PAM and hinder the interaction between AlAc particles and PAM; consequently, gel strength would be affected as well as gelation time. Figure 8 depicts the impact of adding bentonite at various concentrations on the gel strength of 7 wt.% PAM/1 wt.% AlAc with a size of 25 μm. Adding 0.5 wt.% bentonite increased the gel strength of the PAM/AlAc system by ~26% (from 895 Pa for 7 wt.% PAM/1 wt.% AlAc to 1132 Pa) after adding the bentonite. Raising the concentration of bentonite to the range of 1 wt.% did not show a significant impact on the gel strength, whereas incorporating 3 wt.% bentonite reduced the storage modulus of the gel by ~53% (418 Pa).

Figure 9 reveals the influence of adding 1 wt.% bentonite to 7 wt.% PAM/1 wt.% AlAc with a size of 48 μm. The behaviour was different in the case of 48 μm since adding 0.5 wt.% bentonite did not show an enhancement in the gel strength. Moreover, higher concentrations of bentonite considerably decreased the gel strength of the developed gels. It can be deduced that every size of AlAc behaves differently to the addition of the bentonite. These variations could be linked to the difference in the surface area as well as the adsorption of PAM and AlAc on the bentonite surface.\[26\]

### 3.4 Gelation profile

The gelation time is an important factor for the field practice in conformance control treatments and it affects...
the design of the injection process to place the gel in the targeted depth. Figure 10 shows the impact of AlAc particles size on the gelation time of 7 wt.% PAM/1 wt.% AlAc formulation. The smaller the size of the AlAc particles, the faster the gelation. This rapid gelation (about 17 min) is observed when 1 wt.% of 25 μm AlAc is used to crosslink 7 wt.% PAM and attributed to the increased number of crosslinking sites between AlAc and PAM, as the number of the particles and their surface area has been increased after crushing. On the other hand, a larger size of AlAc particles (48 μm) revealed retardation on the gelation of PAM/AlAc because less particles with the lower surface area have crosslinked PAM compared to 25 μm sized particles. A gelation time of 115 min was recorded when 1 wt.% of 48 μm AlAc was used to crosslink 7 wt.% PAM, which is 5.8 times longer than the time required to initiate the gelation when 25 μm AlAc was used in the solution. Using a 65 μm AlAc did not provide a gel at similar conditions, which could be due to particle settling at low PAM concentration.

Figure 11 shows the effect of adding 1 wt.% bentonite on the gelation time of the 7 wt.% PAM/1 wt.% AlAc solution for different AlAc sizes. Bentonite was able to extend the gelation time of the PAM/AlAc system when 25 μm size was used, from 17~40 min. Bentonite hinders the gelation of PAM/AlAc because of PAM adsorption and the positive Al ions on the negatively charged bentonite, therefore reducing the crosslinking sites of PAM/AlAc. Moreover, AlAc particles have been adsorbed on the surface of bentonite because of the high affinity between Al$^{3+}$ and oxygen on the bentonite structure. This phenomenon has been further investigated by molecular simulation in the next section.

### 3.5 Molecular simulation

To understand the proposed mechanism of adsorption, the molecular simulation was employed by studying the adsorption of aluminium ion (Al$^{3+}$) on the clay surface. Kaolinite ($\text{Al}_2\text{Si}_2\text{O}_5\cdot\text{H}_2\text{O}$) was used to represent the clay surface and was retrieved from the materials project database (mp-41152). The VASP (5.4.4.) code was employed and the DFT (density functional theory) calculations used the revised generalized gradient approximation of Perdew, Burke, and Ernzerhof (PBE-GGA) as the exchange-correlation energy for all elements. The building and visualization of the models were done using the QuantumATK Virtual NanoLab. The adsorption of aluminium ion (Al$^{3+}$) on kaolinite was calculated using Equation (1):

$$E_{\text{ads}} = E_{\text{surface} + (\text{Al}^{3+})} - E_{\text{surface}} - E_{\text{Al}^{3+}}$$  \hspace{1cm} (1)

Aluminium ion had a negative value of $-11.854$ eV (Table 2), implying that it has strong adsorption on the clay surface. However, upon the addition of another aluminium ion, the adsorption energy reduced to $-9.25$ eV. This
reduction is due to the electron repulsion of like charges between the aluminium ions (Figure 12). Nevertheless, the negative energy observed upon addition of aluminium ion still implies strong adsorption. The first aluminium ion forms four bonds with the oxygen atoms of the clay surface whereas the added aluminium ion only forms one bond with the oxygen atom of the clay surface. The Al-O bond length (0.185 nm) observed in the added aluminium ion corroborates the decrease in adsorption energy compared to the shorter bond lengths observed in the first aluminium ion bonded to four oxygen atoms. The covalent bonds form two bond angles of 55.9° and 105.3°. This forms an AlAc-like structure, the acetate ion in the AlAc may aid the solubility of the system by forming hydrogen bonds with the hydrogen atoms in the clay structure. On the other hand, PAM adsorption on bentonite is well documented in the literature. Therefore, adsorption of both PAM and Al is likely behind the drop in gel strength. Hence, once bentonite is used in field applications, extra amounts of PAM and Al should be added to compensate for the adsorbed amounts to avoid the drop in gel strength.

4 | CONCLUSIONS

In this study, AlAc with different sizes (d$_{50}$ = 25, 48, and 65 μm) was used to crosslink PAM polymer at 75°C and pH of 5. The impact of AlAc size on the gelation kinetics was investigated as well as the influence of adding bentonite to the formulation. The following conclusions have been made based on the obtained results:

- Reducing the size of AlAc particles significantly improved the stability of the PAM/AlAc system.
- The small size of AlAc (d$_{50}$ = 25 μm) could crosslink PAM at low concentrations with high stable formulations without AlAc settling.
- Decreasing the size of AlAc particles significantly accelerates the gelation process of the PAM/AlAc system and a gelation time of 17 min was obtained for the 7 wt.% PAM at 75°C and pH of 5.
- Bentonite could be used as an additive to delay the crosslinking process of the small size AlAc without significant impact on the gel strength when low concentrations (0.5–1 wt.%) are used.
- The molecular simulation showed that bentonite adsorbs AlAc on its surface which, along with the adsorption of PAM on bentonite, affects the gelation time and gel strength.

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