Theoretical Study of the Use of Branched Polymer Gels as Temperature- and Swelling-Resistant Fluids for Water-Based Drilling Fluids

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ABSTRACT

With the continuous exploration and development of oil and gas resources in deep formations, the use of water-based drilling fluids as a key factor faces severe challenges caused by high temperatures and hydration of soil layers. Therefore, the development of heat- and salt-resistant soil swelling reducer systems has always been of interest. In this study, it was attempted to increase the degree of hydration resistance and thermal stability of the soil by using amino-branched polymer-modified nanoparticles. The interaction mechanism between branched polymer and silica nanoparticles in different states was investigated using density functional theory to determine the best polymer attachment state. The amount of polymer absorption energy in the vertical and horizontal states was 280 and 360 kJ/mol, respectively. The horizontal state prevented water from reaching the soil surface by forming strong hydrogen bonds with the nanoparticle. This amount of absorption energy was higher than that of other similar compounds, which showed that. The thermal stability calculation of the polymer-nanoparticle compound showed that the thermal resistance of this compound is maintained up to temperatures above 280 degrees Celsius. In general, it can be found that branched polymers are a good option for preventing the swelling of drilling wells.

Keywords: Drilling fluids, Nanoparticles, Polymers

1. INTRODUCTION

Drilling fluids, also known as drilling mud, are used to stabilize the wellbore, carry cuttings, and cool and lubricate the drill bit during the drilling process [1-3]. In general, drilling fluids can be classified into water-based drilling fluids (WBDFs), oil-based drilling fluids (OBDFs), and foam drilling fluids based on their composition [4]. WBDFs, a colloidal dispersion consisting of water, bentonite, and various chemical additives, are widely used in drilling engineering due to their relatively economical and environmentally friendly advantages [5].

However, with the rapid growth of global demand for energy resources and the depletion of conventional shallow oil/gas resources, global oil exploration and development is gradually progressing from medium depth to deep, ultra-deep, and other unconventional oil/gas resources. The current WBDFs are not suitable for the complex geological features of deep and ultra-deep wells (such as high temperature, high pressure, high stress, high salt content, etc.) [6,7]. Therefore, the development of water-based drilling fluid technology that is resistant to temperature increase and high salt content is of great importance for the safe, economical, and efficient drilling of deep and ultra-deep wells.

Controlling the hydration of clay surfaces makes the use of water-based drilling fluids challenging for the development of shale formations for fossil resources. Hydration causes severe problems (such as collapse, shrinkage, and sticking) during the use of WBDFs. The initial shale formation may have one to two layers of hydration before WBDFs are pumped through the shale formation during the drilling operation. Further hydration occurs during the drilling operation. This reduces the pressure near the wellbore, which leads to severe problems [8,9].

In recent years, nanomaterials with unique physical and chemical properties such as high-temperature stability, remarkable rheological properties, and filtration properties have shown excellent performance in drilling fluid systems. Various nanomaterials, including mineral nanomaterials (such as graphene oxide, silica, laponite, carbon nanotubes, calcium carbonate, etc.), organic nanomaterials (such as nanospheres, nano gels, nanoemulsions, etc.), and organic/inorganic nanocomposites, have been added to drilling fluids as filter reducers [10]. In addition, nanocomposites prepared by combining mineral nanomaterials and polymers are particularly useful for increasing the dispersibility of nanomaterials and improving the temperature and salt resistance of polymers. For example, a silica nanoparticle-grafted copolymer was prepared by inverse emulsion polymerization that showed excellent filtration performance in high concentrations of Na^+/Ca^{2+} [11]. Bai and colleagues grafted N-isopropyl

acrylamide (NIPAM) onto the surface of Trimethoxy vinyl-modified SiO2 to synthesize a thermally sensitive polymeric plugging agent that showed excellent high-temperature resistance and plugging performance [12].
Branched polymers have attracted a lot of attention due to their unique properties and structural features, such as low viscosity and multiple functional groups. A low-molecular-weight branched polymer can enter the interlayer space of clay and reduce the distance. Based on the low solution viscosity and its ability to minimize the interlayer space of clay, the use of low-molecular-weight branched polyamine to inhibit the hydration of the interlayer surface of clay has become a research branch. In addition, it is necessary to investigate whether the surface hydration of montmorillonite can be inhibited and to what extent. The research results can help to design high-efficiency inhibitors.
In this study, the mechanism of surface hydration inhibition of a nanosilica-modified copolymer gel will be evaluated theoretically using quantum mechanical calculations.

2. Method

First, the structure of the silica nanoparticle (Figure 1) was constructed, which consists of oxygen, silicon, and aluminum atoms. In these calculations, a supercell of 2a2bc was built using the Vesta software. Then, the polymer structure (Figure 2) was built by the GaussView software.

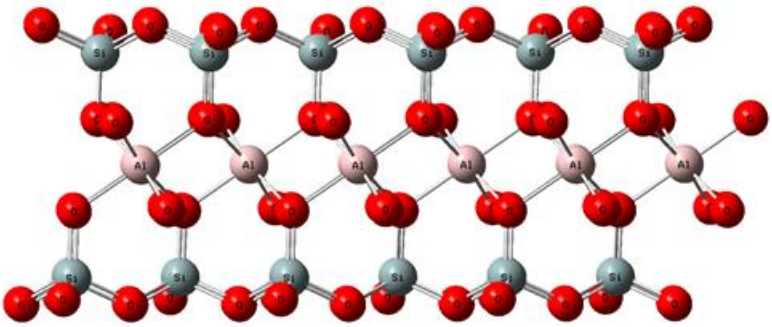

Figure 1- Silica nanoparticles used

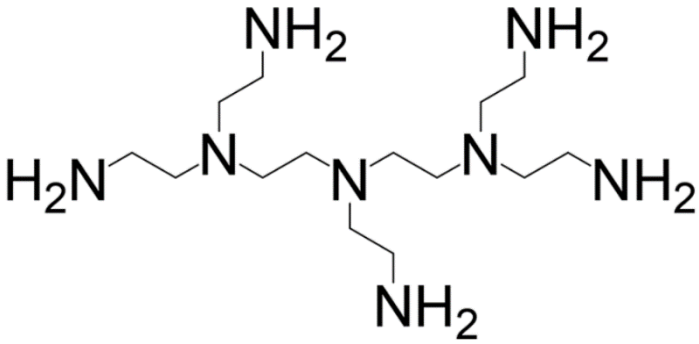

Figure 2- Polymer branch made by GooseView software

Continuing, density functional theory calculations were performed using the Gaussian software. These calculations were performed to optimize the energy of silica and polymer separately and the compound formed by polymer and silica. All calculations were performed at the B3LYP level with the 6-31G* basis set.
The amount of absorbed energy 〖(E〗_ads (Was calculated using formula 1.

In this relationship, in order E_(NP-Polymer) ،E_NP and E_polymer Electronic energy of the nanoparticle composite and polymer , nanoparticle electronic energy, the electronic energy of the polymer .
To find the most stable structure, different orientations were evaluated and various criteria were measured. Following this, and after finding the best state, the thermal stability of the structure was measured.

3. Results and Discussion

According to the results reported in previous studies, the hydration space of nanoparticles decreases when the polymer is added. The water layers between the nanoparticles are eliminated. This is because the polymer chains occupy the space near the surface of the nanoparticles, leaving less space for water to enter.

In this study, the interaction energy between polymer and nanoparticle was compared in different orientations using density functional theory calculations. The goal was to identify the best interaction states.

In this study, the polymer was placed on the nanoparticle in two orientations: vertical (Figure 3) and horizontal (Figure 4). The energy was optimized using a self-consistent field. The results showed that better interactions occurred in the horizontal orientation. In this orientation, the interaction distances were between 2.3 and 3.3 nanometers, while in the vertical orientation, the interactions were between 2.8 and 3.7 nanometers. Additionally, as shown in Figure 4, the number of interactions was higher in this orientation.

A comparison of the interaction types shows that the interactions are of the hydrogen bond type, which is formed between the oxygen atoms on the surface of the nanoparticle and the amino groups of the polymer. These interactions appear to play a significant role in the formation of the interaction and the removal of water from the surface of the nanoparticle. It should be noted that branched polymers form more interactions due to their greater flexibility, which enhances the absorption of the polymer onto the nanoparticles.

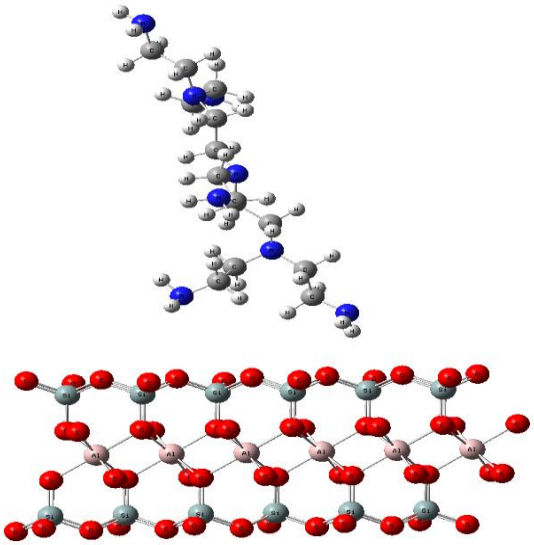

Figure 3- The minimized state of the vertical polymer structure on the nanoparticle

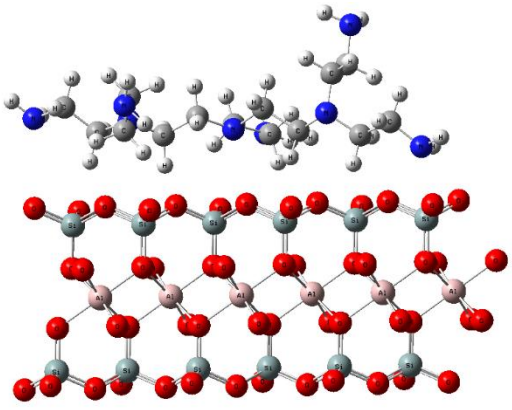

Fig. 4. Minimized structure of the horizontal polymer on the nanoparticle

In Table 1, the calculated absorption energies in two different states are given. As can be seen, the absorption energy for the vertical and horizontal states is -280 and -360 kJ/mol, respectively. These values indicate a strong non-covalent interaction, the main origin of which is the formation of hydrogen bonds. Based on these findings, it can be concluded that the structure in which the polymer is arranged horizontally has a stronger interaction, which can be due to the formation of more hydrogen bonds. This energy value is higher than the reported interaction energy for alkyl amines. These compounds include type one cationic amines (energy of -299.31 kJ/mol) type two amines (-278.33 kJ/mol) and type three amines (-255.05 kJ/mol). Based on these results, it can be concluded that the interaction between the nanoparticle and the polymer can prevent hydration.

Table 1- Polymer absorption energies on the nanoparticle

	Orientation Energy (kJ/mol)
Vertical	-280/18
Horizontal	-360/24

In the following, to evaluate the thermal stability of the nanostructure, temperature changes were applied to the horizontal state, and the results showed that in the horizontal state, the compound formed between the nanoparticle and the polymer is stable up to temperatures higher than 280 degrees Celsius.

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