Supporting Information

Synthesis, characterization and performance evaluation of the environmentally benign scale inhibitor IA/AMPS copolymer

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Table S1.   Main experimental reagents

Reagent name	Manufacturer	Grade
AMPS	Shanghai Aladdin Biochemical Technology Co., Ltd.	AR
IA	Zibo Zhongshi Gerui Biotechnology Co., Ltd.	AR
Sodium hydroxide	Yantai Shuangshuang Chemical Co., Ltd.	AR
potassium bromide	Yantai Shuangshuang Chemical Co., Ltd.	AR
potassium bromate	Yantai Shuangshuang Chemical Co., Ltd.	AR
Potassium iodide	Yantai Shuangshuang Chemical Co., Ltd.	AR
Sodium thiosulfate	Yantai Shuangshuang Chemical Co., Ltd.	AR
Ammonium persulfate	Laiyang Kangde Chemical Co., Ltd.	AR
Sodium chloride	Laiyang Kangde Chemical Co., Ltd.	AR
Soluble starch	Laiyang Kangde Chemical Co., Ltd.	AR
Sulfuric Acid	Laiyang Kangde Chemical Co., Ltd.	AR
Hydrochloric acid	Tianjin BASF Chemical Co., Ltd.	AR
Calcium carbonate	Tianjin BASF Chemical Co., Ltd.	AR
Sodium bisulfite	Sinopharm Chemical Reagent Co., Ltd.	AR
Mercury sulfate	Sinopharm Chemical Reagent Co., Ltd.	AR
Ethanol	Sinopharm Chemical Reagent Co., Ltd.	AR
Sodium sulfate	Sinopharm Chemical Reagent Co., Ltd.	AR
Calcium chloride	Sinopharm Chemical Reagent Co., Ltd.	AR

Text S1. Evaluation of the scale-inhibition performance against calcium carbonate and calcium sulfate [1-3]

The stock solution used in the calcium carbonate inhibition test contained $CaCl_2$ (40 $g \cdot L^{-1}$ Ca^{2+}) and $NaHCO_3$ (48.8 $g \cdot L^{-1}$ HCO_3^-). It is worth noting that the prepared antiscalant stock solution (1000 $mg \cdot L^{-1}$) is always fresh. Add 3 ml of calcium chloride

solution, 5 ml of NaHCO$_3$ solution, and 3 ml of scale inhibitor to the volumetric flask in order. Shake well and transfer to a pre-designed temperature (80℃) water bath for 10 hours. Finally, the solution was cooled to room temperature and the Ca^{2+} concentration in the supernatant was determined using EDTA titration，while a blank test was performed.

According to GB/T16632 national standards, the following steps were used to determine the calcium ion content. Using a pipette, measure 50 ml of the supernatant in an Erlenmeyer flask, add 4-5 drops of hydrochloric acid (volume ratio of concentrated hydrochloric acid and water is 1:1), and then heat to micro-boiling for about 30 seconds. After cooling to room temperature, add 5ml KOH solution with solute mass fraction of 20%. After the addition of the calcein indicator, the test solution showed a green fluorescence, and was titrated with an EDTA standard solution (the concentration of the calibrated EDTA standard solution was 0.0124 mol•L^{-1}). The fluorescence green gradually disappeared and the purple color appeared to be the end point. The calcium ion content (the calcium ion content is based on the mass of calcium carbonate) is calculated as the formula (a).

$$X \text{ (mg·L}^{-1}) = [V_1 \times c(\text{EDTA})/V] \times 100.09 \times 1000 \qquad （a）$$

Where c(EDTA) is the concentration of the EDTA solution (mol•L^{-1}), V$_1$ is the volume of the EDTA solution consumed in the titration (ml), V is the volume of the supernatant taken, and 100.09 is the molar mass of calcium carbonate (g•mol^{-1}).

The stock solution used in the calcium sulfate inhibition test contained CaCl$_2$ (13600 mg•L^{-1} Ca^{2+}) and Na$_2$SO$_4$ (14200 mg• L^{-1} SO$_4^{2-}$). The prepared stock solution was allowed to stand at room temperature for 5 hours. 250 ml of calcium chloride solution and 250 ml of sodium sulfate solution were mixed into a volumetric flask while being adjusted to neutral with sodium hydroxide or hydrochloric acid solution. The cooling water containing different dosages of scale inhibitors was heated at 80℃ for 6 h. Determination of calcium ion concentration by reference to formula (a).

Text S2. Dispersion testing

0.5g of polymer product was added to a 50mL colorimetric tube and deionized water was added to make a 50mL polymer solution. Add 1 g of calcium carbonate powder to the colorimetric tube, cover the lid of the cuvette, and shake vigorously up and down 100 times. Place the colorimetric tube at room temperature for approximately 30 minutes. Accurately pipette 10 mL of the solution into a 250-mL Erlenmeyer flask at 25 mL of the colorimetric tube and add 35 mL of distilled water. Add 10mL of hydrochloric acid solution with a concentration of 0.5mol•L^{-1} and 2-3 drops of phenolphthalein indicator. Finally, titrate the solution in the above conical flask with sodium hydroxide standard solution (0.25mol•L^{-1}) until the red color appears.

Text S3. Determination of intrinsic viscosity and relative molecular mass

Soak the Ukrainian viscometer with chromic acid lotion, then rinse with distilled water 2-3 times, pay attention to repeated cleaning of the capillary part, wash and dry after use. Adjust the temperature of the bath to (30.0±0.1) ℃. Put a hose on the B and C pipes, and place it vertically into the constant temperature bath so that the water surface is completely immersed in the G ball. Pipette 10ml of distilled water and inject it into the viscometer from the A tube and heat for 15 minutes. Use a spring clip to hold the hose on the C tube and use the ear syringe to slowly suck up the solution from the B tube to 2/3 of the D ball. At the same time, loosen the B and C tubes so that the B tube solution flows through the capillary under gravity. Record the time that the liquid surface passes through a scale line to the scale line b, and repeat three times. The average value of the three data measured according to the above method is the outflow time (t_0) of the blank sample.

The concentration of scale inhibitor test solution is 0.005g ml^{-1}. The average value of the three data measured according to the above method is the outflow time (t) of the scale inhibitor test solution. The intrinsic viscosity number was calculated by the following formula (b).

$$\eta = \frac{\sqrt{2(\eta_{sp} - ln\eta_r)}}{\rho} = \frac{\sqrt{2\left[\left(\frac{t}{t_0}-1\right)-ln\frac{t}{t_0}\right]}}{\rho} \qquad (b)$$

Where η_{sp} is specific viscosity, $\eta_{sp} = \frac{t}{t_0} - 1$; η_r is relative viscosity, $\eta_r = \frac{t}{t_0}$;

$\rho(\frac{g}{dL})$ is mass concentration of the scale inhibitor test solution; $t_0(s)$ is the time of standard solution flowing through the viscometer; $t(s)$ is the time of the scale inhibitor test solution flowing through the viscometer.

Text S4. Details of MD simulations

The coupling to the heating bath was carried out by Berendsen method [4], with a relaxation time of 0.1 ps. MD simulation was started by taking initial velocities from a Maxwell distribution. The solution of Newton's Motion Laws was based on following assumptions: periodic boundary condition and time average equivalent to the ensemble average. Integral summation was carried out with a Verlet velocity integrator [5]. The nonbonding interactions in each system, as well as the Van der Waals and electrostatic forces were simulated by an atom-based summation method and the Ewald summation method, respectively, with a cutoff radius of 0.95 nm (spline width: 0.10 nm; buffer width: 0.05 nm). Tail corrections were used to calculate the potential energy contributions from interactions between atoms separated by distances longer than the nonbonding cutoff.

References

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