The Scale Inhibition Performance and Mechanism of Polyepoxysuccinic Acid for Calcium Phosphate

Wu Lei, Wenyan Shi, and Gang Chen

Abstract—The static scale-inhibiting method was employed to investigate the scale inhibition performance of polyepoxysuccinic acid (PESA) on calcium phosphate, and molecular dynamics (MD) method was used to simulate the interactions between PESA and (001), (010) surfaces of hydroxyapatite (HAP, the most thermodynamically stable phase of calcium phosphate) in aqueous solution. The results show that the scale inhibition efficiency of PESA increases as the increase in the concentration and PESA possesses better scale inhibition performance compared with PAA while poor performance compared with POCA. Moreover, PESA molecules adsorb on the surfaces rather than remain in the bulk water in MD simulations and the binding energy of PESA with (010) is significantly stronger (1.8 times) than that with (001) surface, which is mainly provided by hydrogen bonds and coulomb interaction verified by the analysis of radial distribution functions. The adsorption of PESA changes the growth rate of crystal surfaces and leads to changes in the crystal morphology of HAP, according well with the scanning electron microscopy (SEM) results. These suggestions may be useful for the synthesis of new, highly effective scale inhibitors.

Index Terms—Polyepoxysuccinic acid, calcium phosphate, hydroxyapatite, molecular dynamics simulation, static scale-inhibiting method, crystal surface.

I. INTRODUCTION

An impressive set of researches on the precipitation of calcium phosphate have been performed by many researchers [1]–[4]. This is because the importance of calcium phosphate precipitation in diverse areas including pathological biomineral deposits resulting in problems (e.g., dental calculus, arteriosclerosis, urinary calculi, *etc.*), oil and gas production, water purification, energy production technology, waste water treatment processes and industrial water systems, where calcium phosphate precipitation on heat exchanger surfaces could result in decreased efficiency of the system and explosion accidents.

Adding scale inhibitors to the system is the specially common and effective way to prevent the deposition of calcium phosphate. Hydroxyapatite (HAP) is the most thermodynamically stable among different calcium phosphate phases [5], [6]. The growth of HAP could be prevented or slowed with the use of scale inhibitors; in addition, the crystal morphology of HAP could be changed due to the influence of

scale inhibitors. Up to now, the research, development and performance evaluation of new scale inhibitors still mainly rely on experimental and experience extrapolation methods, which will be prone to bring on the waste of time, manpower and material resources. However, the experimental results could not provide us enough microscopic details about how the scale inhibitors interact with the inorganic scale crystal, and the interaction mechanism is still not clear. In contrast, molecular dynamics (MD) simulation can be used to obtain more detailed insights into the scale inhibition mechanism and the effect of scale inhibitors on the morphology of inorganic scale crystal [7]–[9].

Polyepoxysuccinic acid (PESA) is an environment-friendly scale inhibitor synthesized at the beginning of 1990s by Precor & Gamble Company and Betz Company, respectively [10]. PESA is a kind of organic compound which is biodegradable and does not contain nitrogen and phosphorus. According to the characteristics of PESA, such as excellent thermal stability, less amount used and synergistic effect for corrosion inhibition, it is being an important study problem in water treatment field. In China, the synthesis and scale inhibition performance of PESA have been researched since late 1990s, the results indicate that PESA is very capable of controlling calcium carbonate, calcium sulfate and barium sulfate. However, very little is known about the antiscaling property and scale inhibition mechanism of PESA for calcium phosphate scales.

For this purpose, in the present work, the scale inhibition performance of PESA on the precipitation of calcium phosphate was studied by static scale-inhibiting method to explore the effect of scale inhibitor concentration on the scale inhibition performance, and scanning electron microscopy (SEM) was employed to characterize the morphology of HAP to elucidate the role of PESA in the process of crystal growth. On the other hand, the PESA adsorption on the main growth crystal surfaces of HAP in aqueous solution was investigated using Molecular dynamics (MD) simulation to find out the essence of the interaction and the scale inhibition mechanism of PESA. The results provide theoretical guidance to practical applications of PESA.

II. EXPERIMENT

A. Materials

PESA was provided by Changzhou Wujin Water Quality Stabilizer Factory (Jiangsu, China) and was industrial product. Anhydrous calcium chloride, potassium dihydrogen phosphate and sodium tetraborate decahydrate were all analytical reagent grade chemicals.

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B. Static Scale-Inhibiting Method

The static scale-inhibiting method was used to determine the scale inhibition efficiency over a range of concentrations (mg/L) for PESA. Briefly this was as follows:

A simulated water sample containing 250 mg/L (calculated by CaCO_3 concentration) calcium ion and 5 mg/L (calculated by PO_4^{3-} concentration) phosphate was obtained with anhydrous calcium chloride and potassium dihydrogen phosphate, and the pH of the solution was brought to the desired value 9.0 by the careful slow addition of sodium tetraborate decahydrate solution. The scale inhibitor was added to the simulated water sample, and the solution was heated 10 hours at 80 °C. After this stage was completed, the solution was cooled and then filtered. Finally, the concentration of phosphate in the filtrate was measured with spectrophotometry. The scale inhibition efficiency (η) was computed according to the following equation:

$$\eta = (c_b - c_0) / (c_b - c_0) \times 100\% = (I_1 - I_0) / (I_b - I_0) \times 100\% \quad (1)$$

where c_b (I_b) is the concentration (absorbance) of PO_4^{3-} in the simulated water sample (without heating), mg/L, c_0 (I_0) and c_i (I_i) are the concentration (absorbance) of PO_4^{3-} in the filtrate, absence and in the presence of inhibitor, respectively, mg/L.

C. Molecular Dynamics Simulation Method

1) Simulation force field

COMPASS force field [11], available from molecular modeling program Materials Studio 3.0 [12] from Accelrys Software Inc. (USA), was used to simulate the interaction of PESA with HAP crystal surfaces. On the one hand, it is the first *ab initio* force field which has been parameterized and validated using condensed phase properties, in addition to various *ab initio* and empirical data for molecules in isolation. Consequently, this force field enables the accurate and simultaneous prediction of structural, conformational, vibrational, and thermophysical properties for a broad range of molecules in isolation or condensed phases under a wide range of conditions of temperature and pressure. On the other hand, this force field has been successfully employed to investigate the carboxylic polymers [1], [7]. The detailed expressions used to represent the energy surface of COMPASS force field were shown in literatures [11]-[14].

2) Model construction

The models were built with Visualizer module, molecular dynamics (MD) and the energy minimization (EM) calculations were performed on Discover module.

Hydroxyapatite crystals belong to the P63/m space group [15], hexagonal crystal system; the lattice parameters are as follows: $a = b = 0.9424$ nm, $c = 0.6879$ nm, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$. The mode which the surface cells are created from the unit cell of HAP at its cleavage planes was adopted to research the effect of PESA dissolved in water on the growth of (001) and (010) crystal surfaces. The super cells of surface (001) and (010) were extended to 3D periodic super cells of 2.752 nm $\times$ 3.264 nm $\times$ 3.463 nm and 2.752 nm $\times$ 2.827 nm $\times$ 3.888 nm, respectively. Because it is out of the capability of the current simulation technique to take all of these factors into account simultaneously, these variables were changed

step by step. In the present work, the HAP crystal surfaces considered were perfect planes, without defects such as vacancies, steps or kink sites.

The degree of polymerization of PESA was set to 20. The alkyl chains of the polymers are flexible, free to bend and rotate. Therefore, polymers have a variety of configurations, which were continuously converted mutually. Aside from the lowest energy configuration, there were considerable higher energy configurations; however, It was unrealistic to take over all of the possible configurations. With this in mind, the deviation was reduced by increasing the number of configurations, making the simulation results closer to the actual. The torsion angles between the monomers were set to 0° , $\pm 45^\circ$, $\pm 90^\circ$, $\pm 135^\circ$ and 180° ; for each torsion angle, ten configurations were randomly constructed as a set of samples, then eight sets of samples were constructed, specifically, eighty configurations in total for PESA. All the MD simulations of these eighty configurations were carried out at 353 K in the NVT ensemble [16]. MD simulation time was 100 ps and the time step was set to 1 fs; every 5000 steps generated one outcome and 20 frames were generated in total. The configuration of the twentieth frame was optimized to determine the minimum energy using a molecular mechanic (MM) method, the smart minimizer, which combines the steepest descent algorithm, the conjugate gradient algorithm, and the Newton algorithm. The ten lowest energy conformations of the eighty configurations reform a set of samples.

A "liquid layer" consisted of one PESA molecule and two hundred water molecules was added to the simulation box in close proximity to the (001) and (010) surfaces of HAP as starting state. As to the two hundred water molecules, they all moved freely within periodic system boundary. The thickness of vacuum slab along the Z-axis (c) direction was 2.0 nm.

All MD simulations were carried out in the NVT ensemble [16]. The coupling to the heating bath was carried out using the Berendsen method [17], with a relaxation time of 0.1 ps. MD simulation was started by taking initial velocities from a Maxwell distribution. The solution to Newton's Laws of Motion was based on assumptions as follows: periodic boundary condition, and time average equivalent to the ensemble average. Integral summation was carried out with a Verlet velocity integrator [18]. The nonbonding interactions in each system, as well as the Van der Waals force and electrostatic force were computed using 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). When any interaction pair moves more than half this distance, the neighbor list is recreated. Tail corrections were used to calculate the potential energy contributions from interactions between atoms separated by distances longer than the nonbonding cutoff.

Annealing was done using a self-compiled program and the initial temperature of the simulated annealing algorithm was set to 953 K, the temperature decreased once every 50 K, and the MD simulations were performed at each temperature point, till the end temperature 353 K (80 °C), which was the actual application temperature of the scale inhibitors. The time step was set to 1 fs, equilibration stage ran for 100000 fs, and then the production stage also ran for 200000 fs, the data were

collected for subsequent analysis at the same time. The trajectory was recorded every 500 fs.

3) Solvent effect

As the scale inhibitor discussed is used in cooling water circulation system, therefore it is very important to consider the solvent effect on the simulation results. An aqueous environment was included through the explicit inclusion of water molecules in the simulations. In order to model a more realistic system, the whole simulation box included the HAP crystal surface, the “liquid layer” and an additional layer of five hundred water molecules with fixed spatial positions, acting as the water bulk but with the same physical and chemical properties [19]. The schematic view of the starting conformations for H₂O/PESA/HAP surface supramolecular system is shown in Fig. 1.

III. RESULTS AND DISCUSSIONS

A. Effect of the Concentration of PESA on Scale Inhibition Efficiency

The scale inhibition performance of PESA on calcium phosphate scale has been evaluated using the static scale-inhibiting method and was compared with that of commonly used scale inhibitors, such as polyacrylic acid (PAA) and a copolymer of phosphorous acid/acrylic acid/1-acrylamido-2-methylpropanesulfonic acid (POCA). The scale inhibition efficiency of PESA, PAA and POCA for Ca₃(PO₄)₂ with different concentrations is shown in Table I.

TABLE I: SCALE INHIBITION EFFICIENCY OF PESA, PAA AND POCA FOR Ca₃(PO₄)₂

samples	Scale inhibiting efficiency (%) with different concentrations (mg/L)							
	5	10	15	20	25	30	35	40
PESA	7.0	31.2	37.3	45	52.8	65.5	74.6	80.4
PAA	10.0	16.6	19.7	21.3	28.9	30.1	30.7	30.9
POCA	25.4	43.7	49.1	94.4	100	100	100	100

Analysis of Table I indicates that the scale inhibition efficiency of PESA increases as the increase in the concentration. PESA demonstrates poor anti-scale efficiency for calcium phosphate scale at low scale inhibitor concentration, however exhibits better performance at high concentration. PESA shows better scale inhibition

performance compared with PAA while poor performance compared with POCA, this is because POCA contains sulfonic group and hydroxyl group which is beneficial to the scale inhibition efficiency for calcium phosphate scale.

The growth processes of calcium phosphate scale was examined using scanning electron microscopy (SEM), in order to explore the effect of PESA on the growth morphology of HAP crystal and the scale inhibition mechanism of PESA, as shown in Fig. 2.

Fig. 2. The crystal morphology of PESA recorded by SEM.

From the analysis of Fig. 2, it can be known that the shape of HAP was more regular and the particle size was larger, which manifests that the calcium phosphate scale grows quickly. However, adding PESA (10mg/L) to the simulated water sample, the scale became smaller compared with the scale without PESA, which indicates that PESA possesses better dispersing property, making the scale stay in the microcrystal state. Moreover, the shape of HAP is not regular and the scale crystal structure is not obvious, which shows that PESA can adsorb on the crystal surfaces, interact with the surfaces and lead to distortion of crystal lattice. In this paper, the interaction between PESA and the main growth crystal surfaces of HAP was simulated with MD method, intending to investigate the scale inhibition mechanism of PESA for calcium phosphate.

B. Equilibrium Criteria of Interaction between PESA and HAP Crystal Surfaces

The system must reach the equilibrium state before the production runs and the equilibrium of the system can be judged using the equilibrium criteria for temperature and energy [20], that is, when the fluctuations of temperature and energy are in the range of 5%-10%, the equilibrium of the system is ascertained. For the last 15ps during the equilibration period of PESA on the (010) surface of HAP

crystal, the temperature fluctuated between 325K and 377K, which indicates that the temperature reached the equilibrium state because the temperature fluctuated in the setting temperature 353 ± 28 K and the statistical fluctuation of temperature has met the requirement of the temperature criteria. The energy fluctuation curve in the MD simulation of PESA on the (010) surface of HAP crystal for the last 15ps during the equilibration period are shown in Fig. 3.

Fig. 3. The energy fluctuation curve of the binding process of PESA on the (010) surface of HAP.

As shown in Fig. 3, The energy fluctuation curve is in the range of 0.2%-0.3% during the equilibration period of PESA and the (010) surface of HAP crystal, which indicates that simulation system has reached energy equilibration state and the analytical results of the production runs are reliable. Similar conclusions were obtained when analyzing the system composed of PESA molecule and the (001) surface of HAP.

C. Binding Energy of PESA Adsorbed on HAP Crystal Surfaces

Binding energy (E_b) can well describe the intermolecular interaction strength between the scale inhibitors and the scale crystal, which is defined as the negative value of the interaction energy (E_{inter}). E_{inter} can be evaluated by the total energy of the supramolecular system and its corresponding components in the equilibrium state. Therefore, E_b between PESA and HAP crystal surface in aqueous solution can be calculated by the following expression: [21], [22]

$$E_b = -E_{\text{inter}} = E_T - E_{\text{PESA+water}} - E_{\text{surf+water}} + E_{\text{water}} \quad (2)$$

where E_T is the total energy of $\text{H}_2\text{O}/\text{PESA}/\text{HAP}$ supramolecular system, $E_{\text{PESA+water}}$ and $E_{\text{surf+water}}$ are the total energies of the system containing only PESA and water, the HAP crystal surface and water respectively, E_{water} is the total energy of water.

As shown in Fig. 4, PESA molecules adsorbed closely on the HAP crystal surfaces in presence of water after MD simulation, consequently extensive interactions existed between PESA and HAP crystal surfaces and the configurations of PESA were deformed in the process of interaction. The deformation degree of the structure of a molecule is evaluated by deformation energy (E_d).

$$E_d = E_{\text{poly-b}} - E_{\text{poly}} \quad (3)$$

$E_{\text{poly-b}}$ and E_{poly} are single point energy of the polymer molecule being absorbed and being in free status, respectively.

Fig. 4. Equilibrium structures of PESA adsorbing on (001) and (010) crystal surfaces of HAP.

For visualization, average total energies (E_T) of the supramolecular system, single point energies of the constituent parts ($E_{\text{PESA+water}}$, $E_{\text{surf+water}}$ and E_{water}), interaction energies (E_{inter}), binding energies (E_b) and the corresponding deformation energies (E_d) of PESA are presented in Table II (unit: eV).

TABLE II: BINDING ENERGIES BETWEEN PESA AND HAP CRYSTAL SURFACES AND THE CORRESPONDING DEFORMATION ENERGIES OF PESA (EV)

surface	E_T	$E_{\text{PESA+water}}$	$E_{\text{surf+water}}$	E_{water}	E_{inter}	E_b	$E_{\text{poly-b}}$	E_{poly}	E_d
(001)	96974.6	-574.6	97785.8	-324.1	-560.7	560.7	24.4	20.1	4.3
(010)	111633.8	-600.87	112568.6	-675.0	-1008.9	1008.9	25.0	15.6	9.4

As shown in Table II, the interaction energies of both PESA-HAP (001) and PESA-HAP (010) supramolecular systems are negative, which indicates that the combination of PESA with HAP crystal surfaces is exothermic and thermodynamically favourable, in agreement with the illustration of Fig. 4. The more binding energy is, the strong the intermolecular interaction is. The binding energy of PESA with HAP (010) surface is 1.8 times larger than that of PESA with HAP (001) surface, which manifests that the growth of HAP (010) surface was dramatically inhibited by PESA compared with that of HAP (001) surface, leading to changes in the crystal morphology of HAP. The structures of PESA

adsorbed on HAP (001) and (010) surfaces are both distorted strongly.

D. Radial Distribution Function of the Supramolecular System

The radial distribution function $g(r)$ is usually used to describe the degree of atom disorder in the molecule and can give a measure of the probability of finding a pair of atoms at a given distance (r) in a random distribution. The radial distribution function has found applications in structural investigations of both solid and liquid packing, in studying specific interactions such as hydrogen bonding. The $g(r)$ of the superamolecular system is obtained through analyzing the

MD simulation result of PESA with HAP crystal surface. Take the PESA-HAP (010) supermolecular system as an illustration, the radial distribution function of oxygen atoms, hydrogen atoms in PESA with calcium ions, oxygen atoms in HAP (010) surface are shown in Fig. 5, respectively. Similar $g(r)$ graphs can be obtained when analyzing PESA-HAP (001) supermolecular system.

Fig. 5. Radial distribution function of PESA and HAP (010) surface.

Generally, in $g(r) \sim r$ graph, the peak which is within 0.35 nm mainly consists of chemical bond and hydrogen bond, while the peak which is outside of 0.35 nm is mainly composed of the Coulomb and van der Waals forces. As shown in Fig. 5, the first peak of $g(r)_{O-Ca}$ curve appears around 0.275 nm, which is larger than O-Ca electrovalent bond length, 0.239 nm. This indicates that electrovalent bond cannot be formed between oxygen atoms and calcium ions but strong Coulomb forces exist. Analyzing the $g(r)_{H-O}$ curve, there is a sharp peak in $r=0.207$ nm, and it means that the strong hydrogen bonds exist between hydrogen atoms in PESA and oxygen atoms in HAP (010) surface.

IV. CONCLUSION

In this paper, the scale inhibition performance of PESA for calcium phosphate was evaluated by static scale-inhibiting method and the interaction of PESA with HAP was investigated by means of MD simulations and scanning electron microscopy (SEM). The major results can be summarized as follows.

- 1) PESA exhibits better performance for calcium phosphate scale at high scale inhibitor concentration while poor anti-scale efficiency at low concentration and shows better scale inhibition performance compared with PAA while poor performance compared with POCA.
- 2) PESA possesses better dispersing property and leads to the distortion of HAP crystal lattice.
- 3) PESA molecules adsorb on the surfaces rather than remain in the bulk water in MD simulations and the binding energy of PESA with (010) is significantly stronger (1.8 times) than that with (001) surface, which is mainly provided by hydrogen bonds and coulomb interaction verified by analysis of the radial distribution function. The adsorption of PESA molecules change the growth rate of crystal surfaces and lead to changes in the crystal morphology of HAP, according well with scanning electron microscopy (SEM) results.

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