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Experimental Evaluation and Simulation of Potency for Precipitation of Sulfate Particles

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1. ABSTRACT

Water injection into oil reservoirs is mainly used to maintain pressure and increase oil recovery. However, mixing seawater and formation water can lead to mineral precipitation including sulfated particles which can lead to reduced permeability, and blockage of production wells and operating equipment. Therefore, it would decrease the production rate in addition to the cost of dealing with scale formation. In this study, calcium, barium, and strontium sulfate precipitation have been experimentally investigated under static conditions of 90 °C and atmospheric pressure. Hence, for a more detailed analysis of the structure and elemental composition of the precipitated particles, scanning electron microscopy and energy-dispersive X-ray spectrometry were also used. Furthermore, simulation software of Aspen Plus and PHREEQC were employed to confirm the accuracy and precision of the experimental data via a reasonable agreement between experimental and simulated results which showed that the precipitation potential was from higher to lower for calcium sulfate, strontium sulfate, and barium sulfate.

Keywords: Aspen Plus, PHREEQC, High-temperature Static Test, Precipitation, Sulfated Scales.

2. INTRODUCTION

Seawater injection is commonly used to maintain pressure of oil reservoirs which may lead to higher oil recovery [1-3]. Nevertheless, the incompatible mixing of seawater and formation water can lead to mineral precipitation such as calcium, barium, and strontium sulfates, which in long time would cause lower permeability, blockage in production wells and equipment which comes with extra costs for operation and remedial measures[4-6]. Supersaturation with scale-forming salts caused by changes in operating conditions in which water exists can cause scale precipitation [7]. These include, but not limited to, mixing ratio, temperature, and ion concentration[8, 9]. Experimental and theoretical approaches could be applied to predict the mass of mineral-precipitated particles. In this study, the precipitation of calcium, barium, and strontium sulfates was investigated experimentally (high-temperature static tests) in addition to the simulation tools of Aspen Plus and PHREEQC. Moreover, a scanning electron microscope (SEM) and X-ray energy diffraction (XRD) spectrometer were used for a more detailed analysis of the morphology and elemental composition of the precipitated particles, respectively.

3. MATERIALS AND METHODS

3.1. Materials

To achieve the target ionic solutions, various solutions were prepared by dissolving proper salts in deionized water. Table 1 provides the specific concentrations of the ions and the corresponding salt quantities used for the preparation of these solutions.

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Table 1. Composition of the investigated solutions

Solution	Ion	Ion concentration (mg/L)	Salt used	Mass of salt (g/L)
Cationic	Ca^{2+}	2000	$CaCl_2.2H_2O$	7.723
	Ba^{2+}	296	$BaCl_2.2H_2O$	0.504
	Sr^{2+}	771	$SrCl_2$	1.468
Anionic	SO^{2-}	2960	Na_2SO4	4.376

3.2. Experimental method

Laboratory static jar tests were conducted over a period of seven days to evaluate the potential for precipitation of calcium, barium, and strontium sulfates. Synthetic solutions, as shown in Table 2, were prepared to simulate different ion compositions, with each mixed solution tested for its calcium, barium, and strontium sulfate scaling tendencies at 90°C and atmospheric pressure. After 7 days, vacuum filtration was carried out using 0.2 µm cellulose nitrate filters to separate and weigh the precipitated particles, allowing for an assessment of precipitation potential. Furthermore, the scanning electron microscope (SEM) was used to discern the surface morphology of the precipitated crystals, as well as the X-ray diffraction (XRD) which was employed to study the elemental composition of the crystals.

Table 2. Experimental conditions for precipitation of calcium, barium, and strontium sulfates

Precipitate particles type	Temperature (°C)	Pressure (atm)	Final volume (L)	Mixing ratio cationic: anionic (%)	Time (day)
Calcium sulfate	90	1	0.2	40:60	7
Barium sulfate	90	1	0.2	90:10	7
Strontium sulfate	90	1	0.2	70:30	7

4. SIMULATION APPROACH

Advanced simulation methods using PHREEQC and Aspen Plus were employed to predict the mass of various investigated precipitated particles by similar replicating the experimental conditions. The aforementioned simulation tools provided insights into both thermodynamic and kinetic aspects, respectively. Although two simulation approaches are differently considered, the simplifying assumptions including of the stochiometric reactions could facilitate the understanding of precipitation processes.

5. RESULTS AND DISCUSSION

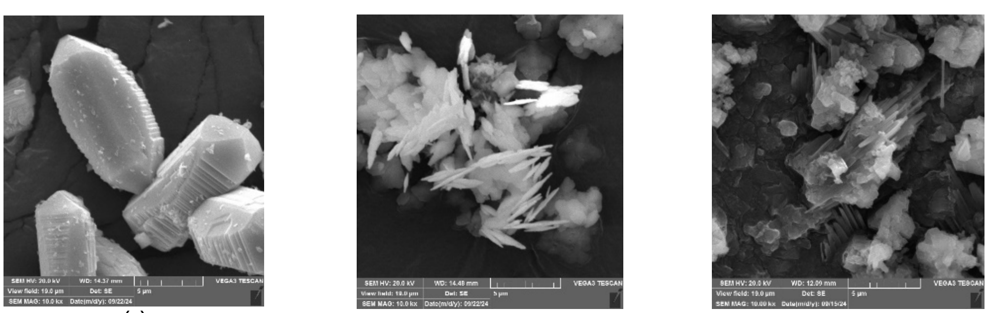
5.1. Experimnetal results

The experimental findings shown in Table 3 indicate that calcium sulfate exhibited the highest precipitation potential, followed by strontium sulfate and barium sulfate under conditions as outlined before.

SEM images revealed distinct morphologies for each precipitate, highlighting differences in crystal growth patterns, while EDX analysis confirmed the expected elemental compositions. According to Fig. 1, the needle-like structures of calcium sulfate crystals (Fig. 1a) indicate a high sequestration rate, attributed to elevated calcium ion concentrations that promote the growth of larger and more stable crystals. The distinct morphologies of barium sulfate (Fig. 1b) featuring regular dense-flake formations and strontium sulfate (Fig. 1c) displaying polyhedral and sharp cone structures.

Table 3. Mass of precipitated sulfate particles at 90°C from the experimental conditions

Precipitate type	Calcium sulfate	Barium sulfate	Strontium sulfate
Mass of precipitated particles per liter of final mixed solution (gr)	15.84	0.45	1.10



(c) (b) (a)

Figure 1. Morphology of precipitated particles from SEM analysis: a) calcium sulfate, b) barium sulfate, c) strontium Sulfate

5.2. Simulation results

5.2.1. Aspen Plus

Based on the simulation process, Table 4 shows the mass of precipitated particles at atmospheric pressure and 90°C per liter of solutions after 7 days, resulted by Aspen Plus. The results indicate that calcium sulfate has a significantly higher precipitation rate compared to barium and strontium sulfate, consistent with experimental data (Table 3). Differences in mass between experimental and simulated results are likely due to simplifications in the simulation. The effect of increasing temperature on precipitation is such that calcium sulfate increases with temperature, while barium sulfate decreases due to increased solubility, and strontium sulfate shows a trend similar to calcium sulfate.

Table 4. Mass of precipitated sulfate particles at 90°C resulted by Aspen Plus

Precipitate type	Calcium sulfate	Barium sulfate	Strontium sulfate
Mass of precipitated particles per liter of final mixed solution (gr)	1.1346	0.4824	1.1265

5.2.2. PHREEQC

PHREEQC simulation results also confirmed the experimental and Aspen Plus simulated findings. Table 5 shows precipitation mases at 90°C under conditions similar to the experiments, where calcium sulfate shows the highest potential of precipitation, aligning with both experimental and Aspen Plus results. The influence of temperature on precipitation for calcium, barium, and strontium sulfates in PHREEQC closely matches the patterns observed in Aspen Plus findings, reinforcing the accuracy of both simulation tools. Furthermore, the calculated error between Aspen Plus and PHREEQC results showed relative errors of 12% for calcium sulfate, 6% for barium sulfate, and 2% for strontium sulfate, demonstrating reasonable agreement with the experimental data.

Table. Mass of precipitated sulfate particles at 90°C from the PHREEQC simulator

Precipitate type	Calcium sulfate	Barium sulfate	Strontium sulfate
Mass of precipitated particles per liter of final mixed solution (gr)	1.1021	0.4515	1.1158

6. CONCLUSION

The main findings of this study are as follows:

- The results showed a reasonable agreement between experimental and simulated approaches which would validate each other so that the precipitation potency from higher to lower for calcium sulfate, strontium sulfate, and barium sulfate were gained. Understanding the interactions between temperature, solubility, and precipitation is crucial for accurate prediction of scaling behavior.
- Higher initial concentrations of cations significantly increased the precipitation rate, with calcium sulfate showing the most pronounced effect.
- SEM analysis revealed distinct morphologies for each sulfate type: calcium sulfate formed as needle-like crystals, barium sulfate as dense flakes, and strontium sulfate as polyhedral cones.
- Simulation results indicated that as the temperature rises, precipitation of calcium and strontium sulfates increases, while barium sulfate precipitation decreases, reflecting their unique solubility characteristics across temperature ranges.

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