

Appendix A. Supplementary data

Text S1 Synthesis of CaO₂ nanoparticles.

The synthesis of CaO₂ nanoparticles involved the following steps: 12g CaCl₂ and 1.2 g CTAB were dissolved in 500 mL distilled water, and slowly add ammonia solution to the stirred mixture to raise the pH to 10. Then 60 mL of 30% H₂O₂ was added to the mixture by rate of 1mL / min. The preparation procedure was carried out in a continuously stirred opened 1000 mL glass beaker at room temperature. The stirrer velocity was kept constant for all the experiments. After 1 h of stirring, a clear and colorless to yellowish solution was obtained. In order to precipitate the product, 1mol/L NaOH was added to raise the solution pH to 11. The white precipitate was separated by centrifuge and after the centrifugation process the powder was washed three times by anhydrous ethanol. Finally, the resultant precipitate was dried by N₂ at room temperature. Fig. S1(a) shows the SEM images of a typical CaO₂ nanoparticles sample. As seen in Fig. S1(a), the nanoparticles are of uniform spherical shape and approximately 20–80 nm in diameter. Chemical composition of the CaO₂ nanoparticles was determined by XRD. The result is shown in Fig. S1(b), the four dominant peaks: $2\theta = 29.4, 35.5, 47.3, 52.6$ match to the XRD of CaO₂ (JCPDS-PDF: 03-0865). The XRD result strongly proved that the CaO₂ nanoparticles compound was formed by this procedure.

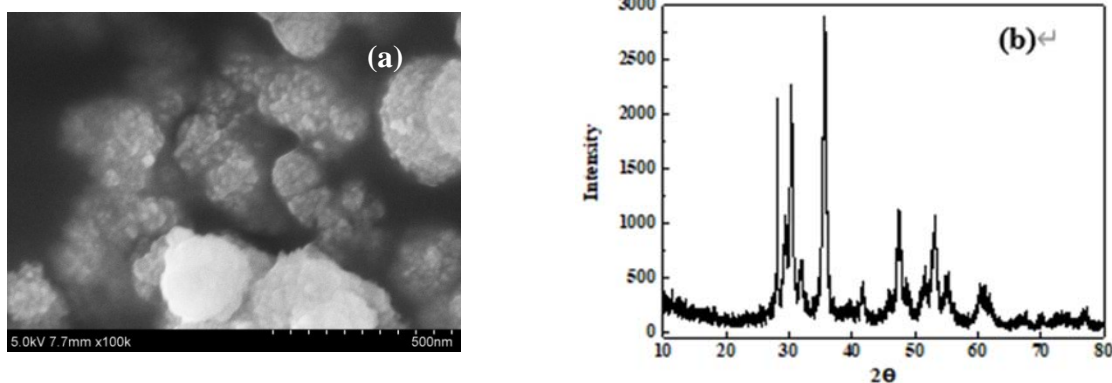


Fig. S1. (a) SEM images of CaO₂ prepared. (b) XRD of CaO₂ prepared.

Text S2:The methods of intermediate products detection by GC-MS and LC-MS

For GC/MS, samples (200 mL) were collected at different reaction times. First, the samples were extracted three times with ethyl acetate and then dried using anhydrous sodium sulfate. The samples were then concentrated in vacuo at 65°C. After the pretreatment step, 1 μ L of the sample was injected in splitless mode. The oven temperature was initiated at 40°C and held for 3 min, and then increased to 200°C at 20 °C/min and held for 5 min, after that the temperature was increased to 250°C at 10°C/min and held for 5 min. The flow rate of the carrier gas helium was 1.0 mL/min. Mass spectra were obtained in EI mode with an electron energy of 70 eV. For LC/MS, 20 μ L of the extract dissolved in acetonitrile was automatically injected into the LC-MS system. The eluent was the same as that used for HPLC and the flow rate was 0.2 mL/min. The MS spectra were acquired over a m/z range of 40–200 in negative scan mode.

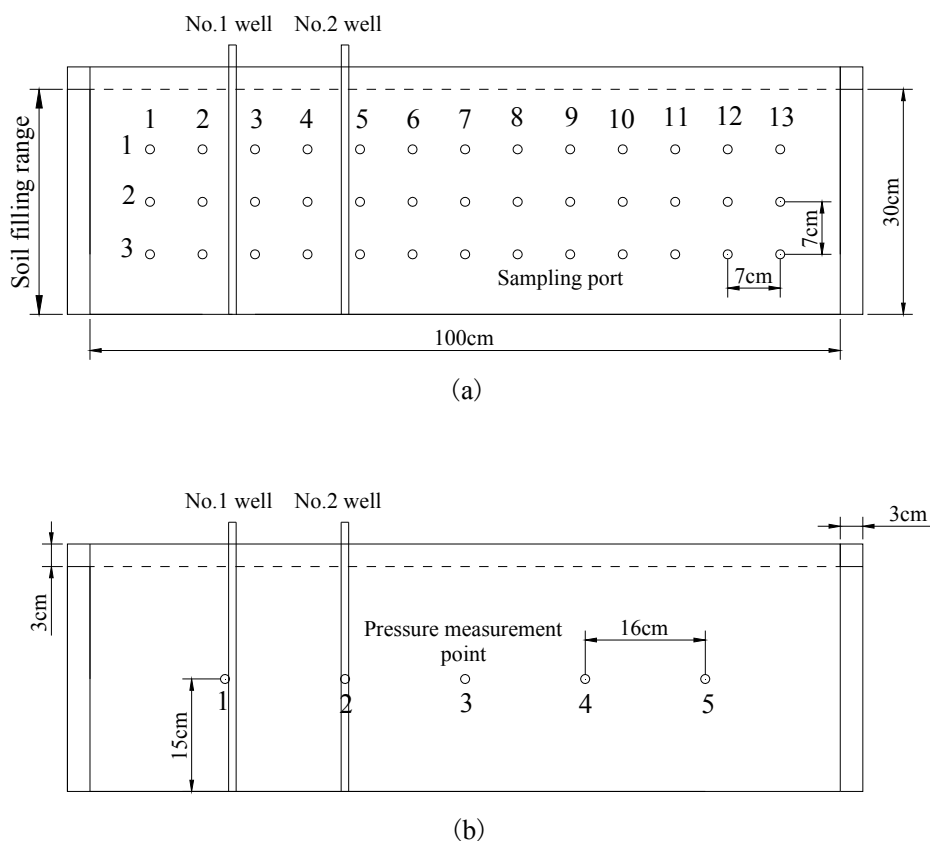


Fig. S2. The schematic diagrams of tank experiments for CaO₂ reaction zone. (a is the front; b is the back)

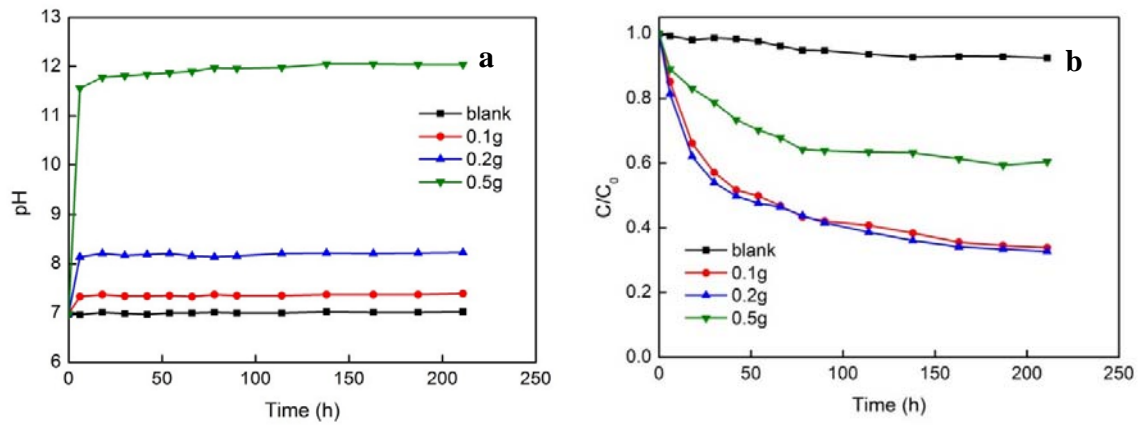


Fig. S3. (a) The 2,4-DCP degradation curves obtained at different CaO₂ concentrations; (b) The change curve of pH with time in the system. Experimental conditions: 2,4-DCP = 30 mg/L, Fe²⁺ = 3 mg/L, initial pH = 7.0.

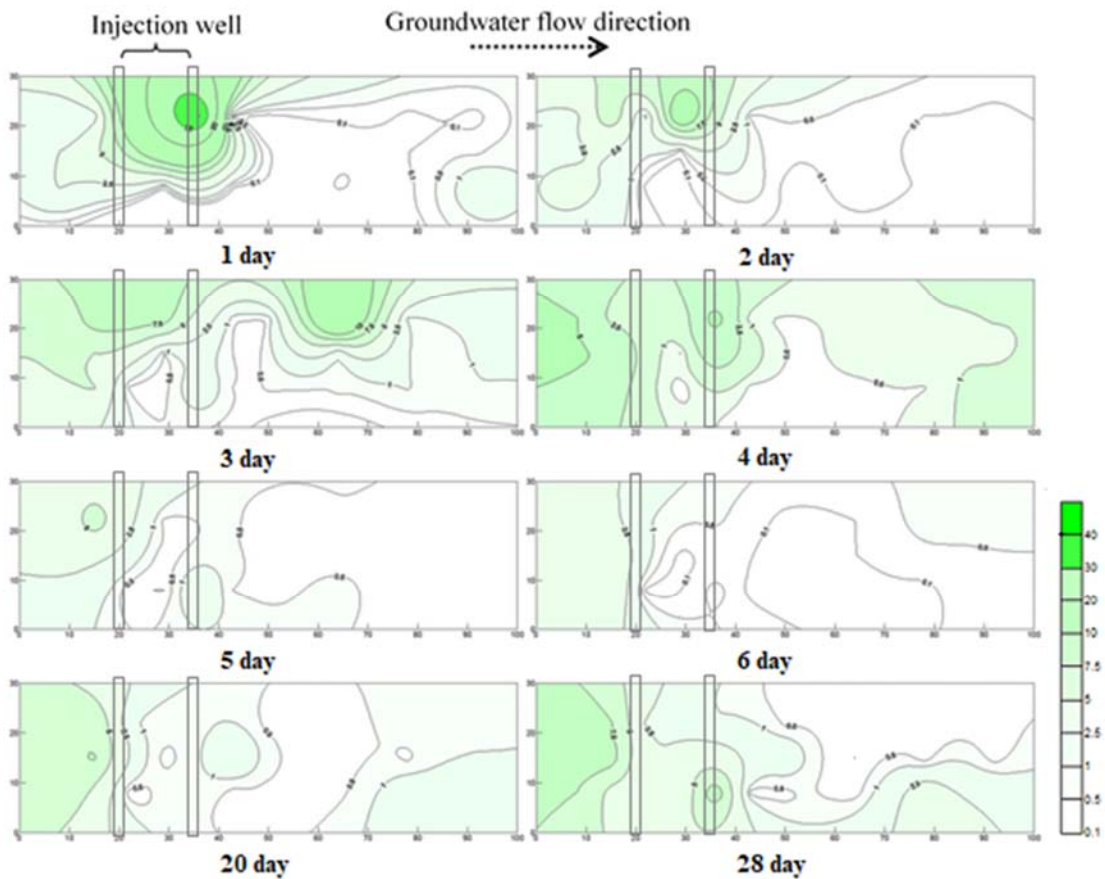


Fig. S4. Change in H₂O₂ concentration in the simulated tank with time.

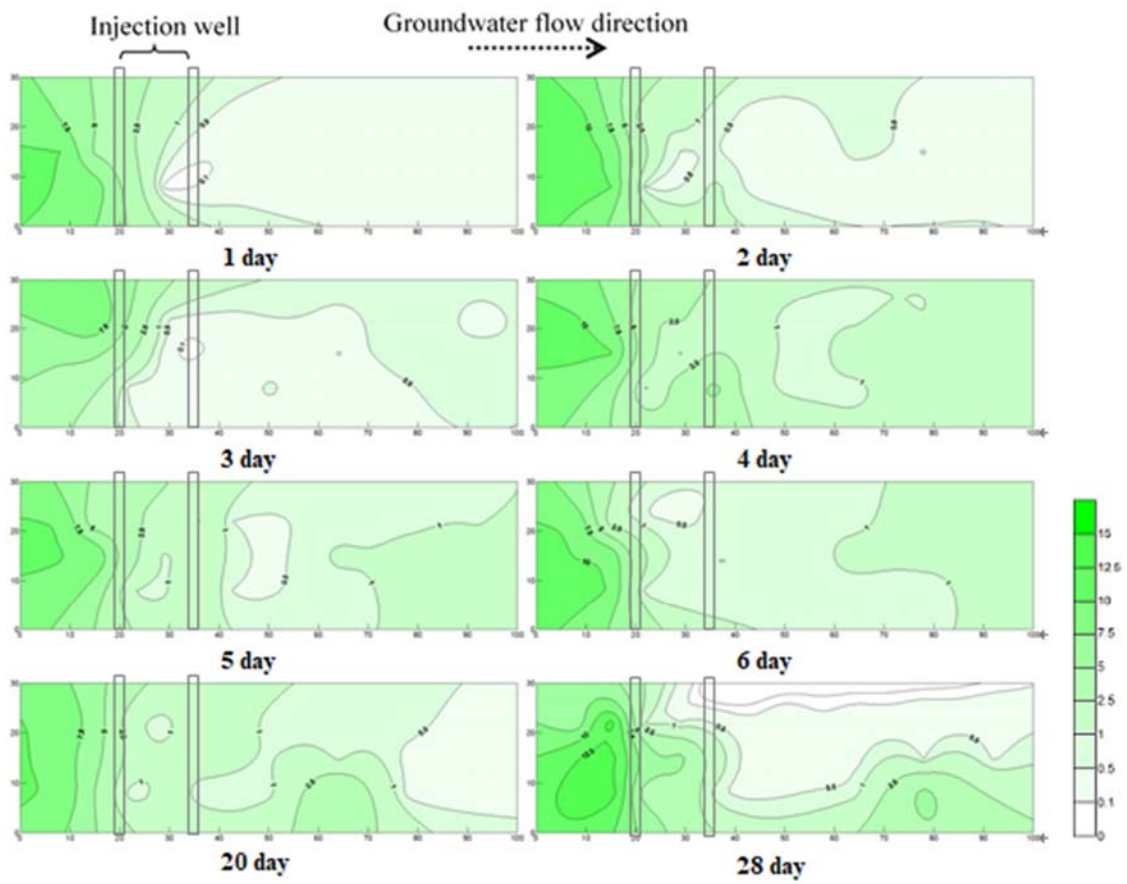


Fig. S5. Change in iron ion concentration in the simulated tank with time.

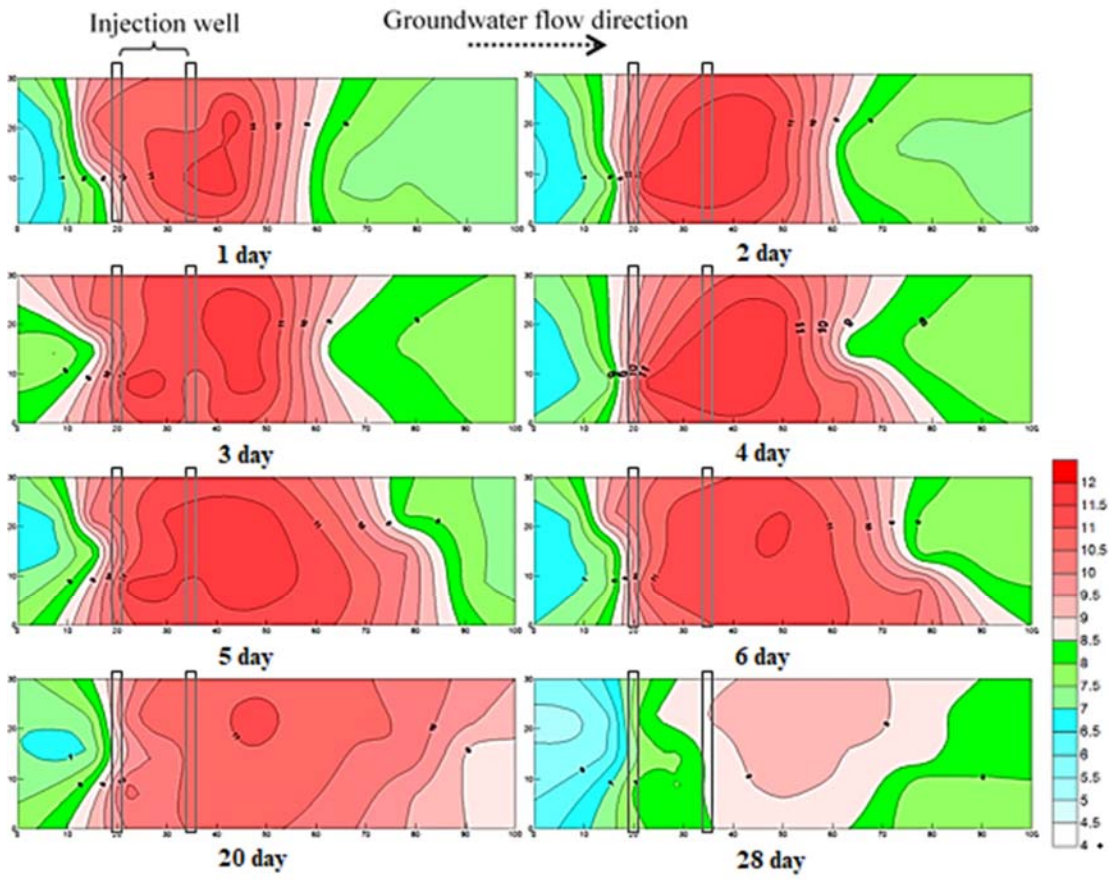


Fig. S6. Change in pH concentration in the simulated tank with time.