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Thermochemical Sulfate Reduction Modeling and Its influence on H_2S concentrations and Porosity of Carbonate Reservoirs

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Summary

Thermochemical sulfate reduction (TSR) stands as a crucial process in naturally producing elevated concentrations of hydrogen sulfide (H_2S) within carbonate reservoirs. The presence of H2S holds significant importance in reservoir management, facility design, and operational safety within the oil industry. Despite extensive research on TSR in various carbonate fields, uncertainties persist regarding the factors influencing variations in H_2S concentrations and changes in reservoir quality during TSR reactions. In addressing this, we have formulated a diagenetic model based on a reactive transport model (RTM) to quantitatively simulate the TSR process. This model is capable of simulating hydrocarbon consumption, the generation of H_2S and CO_2, as well as the dissolution and precipitation of minerals throughout the TSR process. Furthermore, it enables the quantification of the associated modifications to reservoir quality.

Theory / Method / Workflow

The Puguang gas field, a significant discovery in southwest China, has undergone extensive examination, offering an ideal scenario for the application of a reactive transport approach due to well-explored geological backgrounds and the availability of abundant data (Worden and Smalley, 1996; Cai et al., 2010). We selected two wells, PG-2 and PG-6, within the Puguang gas field for the development of a 1D RTM to simulate the TSR process. The modeled well sections were 4776–5196 m for PG-2 (420 m) and 4818–5398 m for PG-6 (580 m).
The RTM utilized PHREEQC v3.6, developed by the U.S. Geological Survey, incorporating thermodynamic equilibrium reactions for gas-water-rock interactions and kinetic reactions for sulfate reduction. The modeling approach incorporated present-day log-based well depth and thickness, paleo mineralogy assemblages, paleotemperature in the late Jurassic, and hydrostatic pressure(Lu et al., 2020, 2022).
TSR is considered as a kinetic reaction with a constant rate of 1.13×10^{-13} mol/s at 190 ◦C based on the reaction rate of CH_4 in the presence of $MgSO_4$ ion pair from He et al. (2019) for the following reaction:

$$CH_4 + CaSO_4 \text{ (anhydrite)} = H_2S + H_2O + CaCO_3 \text{ (calcite)} \quad (1)$$

Results, Observations, Conclusions

The modeling outcomes reveal that the local efficiency and scope of TSR reactions are influenced by the lithological components and gas saturation within the reservoir. The presence of abundant effective anhydrite, acting as the oxidizing agent, and hydrocarbon, serving as the reducing agent, plays a pivotal role in the generation of H_2S and calcite cements (Figure 1). This suggests that the abundance of anhydrite is a critical factor governing the extent of TSR reactions and the distribution of H_2S. Observations from petrography imply a positive correlation between the increase in H_2S and the dissolution of effective (or reactive) anhydrite. Consequently, it is inferred that the concentrations of H_2S in the targeted reservoir interval are primarily influenced by the availability of effective anhydrite within this specific interval.

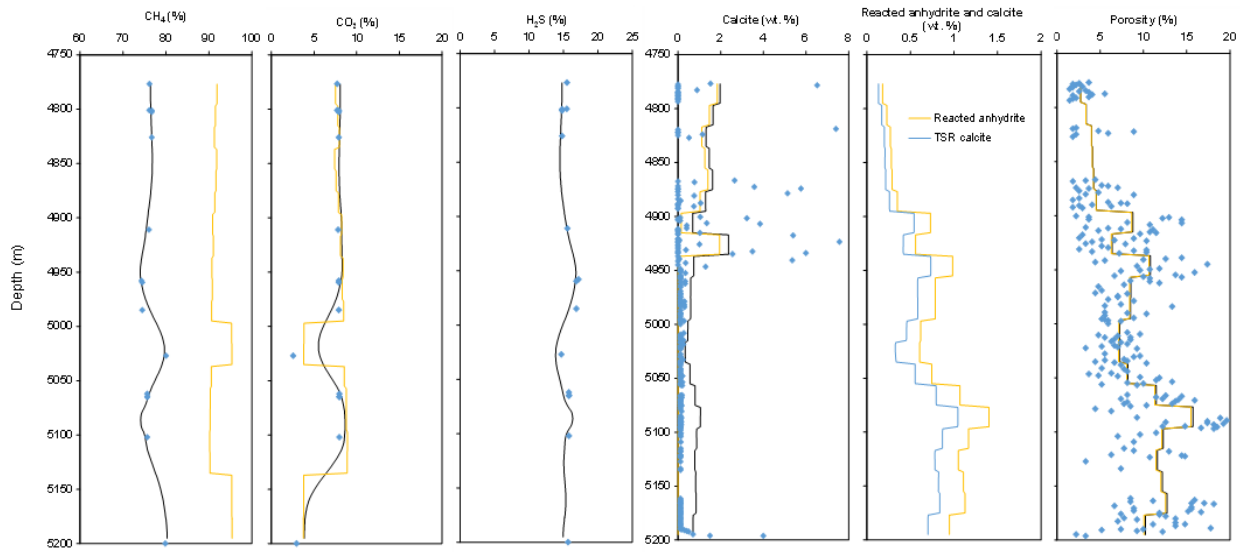

Figure 1. Modeling results for Well PG-2 (black lines) compared with the observed values (blue points).

Modeling result also shows that the porosity generation due to the TSR reactions is insignificant, around 0.23%, probably because the impacts of anhydrite dissolution and calcite precipitation on porosity offset each other. As calcite is 36.934 cm^3/mol and anhydrite is 45.94 cm^3/mol, the net increase of porosity is calculated as 9 cm^3 per mol anhydrite (mole-to-mole replacement).

Novel/Additive Information

The TSR modeling is a powerful tool to describe the organic-inorganic interactions and their impacts on both non-hydrocarbon (H_2S and CO_2) generation and reservoir qualities during TSR process. The modeling can also provide a quantitative estimation of H_2S concentration and the consumption of hydrocarbon in TSR, which would be useful for evaluating H_2S risk and mapping its distribution to optimize the exploration and management on carbonate reservoirs.

In future studies, combining RTM and basin modeling has the potential to enhance the predictive capabilities of the modeled TSR system for both reservoir and petroleum quality. RTM modeling relies on inputs from a comprehensive geological model, rock and fluid properties, and the thermal and burial history of the specific system under consideration. Basin modeling, particularly in providing crucial inputs such as fluids, thermal and burial history, and boundary conditions, can complement RTM. The outcomes of RTM can then be integrated into basin modeling, improving the quantification of diagenetic processes and aiding in the prediction of non-hydrocarbon gas inputs in the reservoir.

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