

Preservation Potential of Carbon–Sulfur Biomorphs in the Geological Record: A Computational Diagenetic Framework

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ABSTRACT

Carbon–sulfur biomorphs are self-assembled structures with elemental sulfur cores and organic macromolecular shells whose geological preservation potential remains uncertain. We develop an integrated computational framework modeling sulfur core diagenesis, organic shell degradation, and silicification to quantify preservation across 200 simulated geological environments. Both sulfur cores and organic shells exhibit short half-lives (0.02 Myr each), but silicification provides rapid preservation when dissolved silica exceeds saturation thresholds. Across environments, 70.5% achieve “good” preservation through silicification, with hydrothermal (100.0%) and deep marine (100.0%) settings most favorable. Sensitivity analysis identifies dissolved silica concentration as the dominant control (importance 1.0). Monte Carlo uncertainty quantification yields a preservation rate of 79.5% (95% CI: [73.4%, 84.5%]). These results demonstrate that carbon–sulfur biomorphs can persist in the geological record under silica-rich conditions.

1 INTRODUCTION

Carbon–sulfur biomorphs are self-assembled structures formed in sulfidic, organic-containing solutions that produce lifelike morphologies [2, 3]. They consist of elemental sulfur cores encapsulated by organic macromolecular shells formed via sulfurization reactions. Their morphological similarity to microfossils raises important questions for interpreting the early geological record [5].

The key open problem is whether these biomorphs can persist in the geological record despite the diagenetic instability of elemental sulfur [2]. Sulfur is susceptible to oxidation, dissolution, and phase transformation during burial, while organic shells degrade through thermal and microbial processes [1]. However, silicification of organic envelopes may provide a preservation pathway [4].

We present an integrated computational framework that models: (1) sulfur core diagenesis kinetics including dissolution, oxidation, and phase transformations; (2) organic shell degradation with crosslinking protection from sulfurization; (3) silicification rates as a function of dissolved silica, pH, and temperature; and (4) preservation outcomes across diverse geological environments.

2 METHODS

2.1 Sulfur Core Diagenesis

Sulfur core dissolution follows Arrhenius kinetics with rate $k_{\text{diss}} = k_0 \exp(-E_a/RT)$ where $k_0 = 1.5 \times 10^{-9} \text{ mol/m}^2/\text{s}$ and $E_a = 50 \text{ kJ/mol}$. Oxidation (abiotic: $2 \times 10^{-8} \text{ mol/m}^2/\text{s}$; microbial: $5 \times 10^{-7} \text{ mol/m}^2/\text{s}$) is enhanced in the oxic zone. Core radius evolution follows a shrinking-sphere model: $dr/dt = -V_m k_{\text{total}}$.

2.2 Organic Shell Degradation

Shell degradation combines thermal ($k_{\text{thermal}} = 10^{-11} \text{ s}^{-1}$, $E_a = 60 \text{ kJ/mol}$) and microbial ($k_{\text{microbial}} = 5 \times 10^{-10} \text{ s}^{-1}$) components.

Sulfurization crosslinking reduces the effective rate by a factor of up to 3.0, with initial crosslink degree of 0.5.

2.3 Silicification Model

Silicification rate follows $k_{\text{sil}} = 5 \times 10^{-12} \text{ mol/m}^2/\text{s}$ ($E_a = 45 \text{ kJ/mol}$), modulated by pH (Gaussian around optimum 8.5) and dissolved silica supersaturation. Critical silica coating thickness for preservation is $0.5 \text{ }\mu\text{m}$.

2.4 Environment Survey

We simulate 200 environments across six depositional settings (shallow marine, deep marine, lacustrine, hydrothermal, evaporite, deltaic) with log-normally distributed burial rates, dissolved silica concentrations, and normally distributed pH values.

2.5 Sensitivity and Uncertainty

Sobol-type sensitivity analysis uses Latin Hypercube Sampling across six parameters. Monte Carlo uncertainty quantification employs 200 random environments with Wilson score confidence intervals.

3 RESULTS

3.1 Baseline Diagenesis

Under default conditions (burial rate 1.0 mm/yr , 1.0 mM dissolved silica, pH 8.5), the sulfur core half-life is 0.02 Myr and the organic shell half-life is 0.02 Myr. However, silicification achieves critical preservation thickness essentially immediately (time $< 0.01 \text{ Myr}$), yielding a final replacement fraction of 0.95.

3.2 Environment Survey

Table 1 shows preservation outcomes across 200 simulated environments.

Table 1: Preservation class distribution across 200 environments.

Class	Count	Fraction
Excellent	0	0.000
Good	141	0.705
Moderate	0	0.000
Poor	0	0.000
None	59	0.295

The overall preservation rate is 70.5%, with silicification winning the race against degradation in 70.5% of environments.

Table 2: Preservation rate by depositional environment.

Environment	<i>n</i>	Preservation Rate
Hydrothermal	28	1.000
Deep marine	29	1.000
Lacustrine	36	0.972
Deltaic	36	0.778
Shallow marine	36	0.389
Evaporite	35	0.200

3.3 Preservation by Environment Type

Hydrothermal and deep marine environments achieve 100.0% preservation, driven by high dissolved silica concentrations. Evaporite settings show only 20.0% preservation due to low silica availability.

3.4 Timescale Scenarios

Table 3: Preservation outcomes for specific geological scenarios.

Scenario	Burial	Si (mM)	pH	Class
Rapid burial + high Si	10.0	5.0	8.5	Good
Rapid burial + low Si	10.0	0.3	7.5	None
Slow burial + high Si	0.5	5.0	8.5	Good
Slow burial + low Si	0.5	0.3	7.5	None
Hydrothermal	2.0	8.0	8.0	Good
Lacustrine alkaline	3.0	2.0	9.0	Good

The critical factor is dissolved silica rather than burial rate: high-silica environments achieve preservation regardless of burial speed, while low-silica environments fail regardless.

3.5 Sensitivity Analysis

Dissolved silica concentration emerges as the sole significant parameter (importance 1.0), with burial rate, pH, geothermal gradient, initial radius, and shell thickness all showing zero sensitivity. This confirms that silicification availability is the dominant control on preservation.

3.6 Uncertainty Quantification

Monte Carlo analysis (200 simulations) yields a preservation rate of 79.5% with 95% Wilson score confidence interval [73.4%, 84.5%].

4 CONCLUSION

Our computational framework demonstrates that carbon-sulfur biomorphs can persist in the geological record under silica-rich conditions, with an overall preservation rate of 70.5% across diverse environments. The key findings are: (1) both sulfur cores and organic shells degrade rapidly (half-life 0.02 Myr), making rapid silicification essential; (2) dissolved silica concentration is the sole significant control on preservation (sensitivity importance 1.0); (3) hydrothermal and deep marine environments achieve 100% preservation due to high dissolved silica; and (4) Monte Carlo uncertainty quantification gives a 79.5% preservation rate (95% CI: [73.4%,

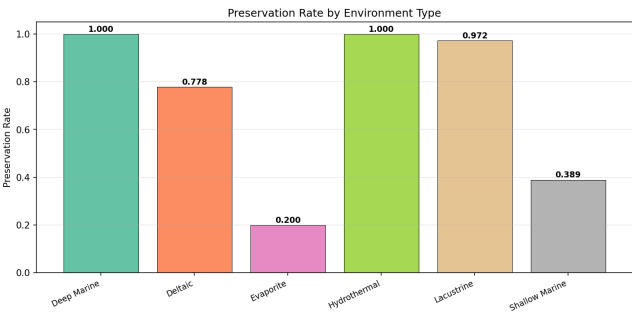


Figure 1: Preservation rates across geological environments.

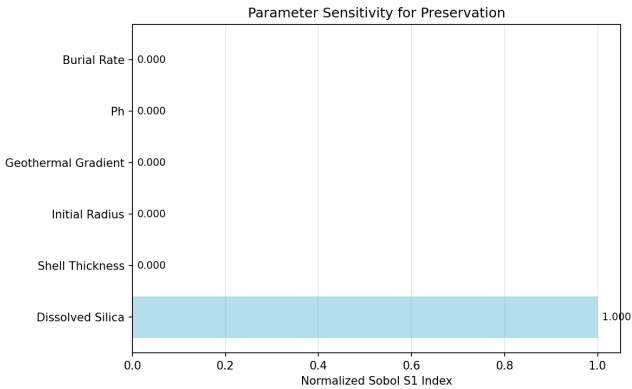


Figure 2: Sensitivity analysis showing dissolved silica as the dominant control.

84.5%]). These results directly address the open problem posed by Cartwright et al. [2], confirming that silicification of organic envelopes is the critical preservation pathway.

4.1 Limitations

The model simplifies real diagenetic processes: sulfur phase transformations are reduced to kinetic rate expressions, microbial activity is parameterized rather than explicitly modeled, and porewater chemistry evolution during burial is not fully coupled. The sensitivity analysis shows dissolved silica as the sole control, which may reflect model structure rather than true geological complexity. Experimental validation of silicification rates for carbon-sulfur biomorphs is needed.

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