

Supplement to Henkel et. al., “Stable iron isotope signals indicate a “pseudo-abiotic” process driving deep iron release in methanic sediments”

Table S1: Reactions implemented into the diagenetic model and rate expressions.

Reactions		
$\text{CH}_2\text{O} + 4\text{Fe}(\text{OH})_3 \rightarrow \text{HCO}_3^- + 4\text{Fe}^{2+} + 3\text{H}_2\text{O} + 7\text{OH}^-$	*	R1
$\text{Fe}(\text{OH})_3 + 2\text{HS}^- \rightarrow \text{FeS}_2 + 2\text{OH}^- + \text{H}_2\text{O} + 0.5\text{H}_2$		R2
$\text{Fe}^{2+} + 2\text{HS}^- \rightarrow \text{FeS}_2 + \text{H}_2$		R3
$\equiv \text{S} - \text{H}^0 + \text{Fe}^{2+} + \text{HCO}_3^- \rightarrow \equiv \text{S} - \text{Fe}^+ + \text{CO}_2 + \text{H}_2\text{O}$	**	R4
Rate expressions		
$R_1 = R_G = -k_1 G = -k_1 G_0 \exp(-k_1 z/\omega)$		E1
$R_2 = k_2 [\Sigma \text{H}_2\text{S}]$		E2
$R_3 = k_3 [\text{Fe}^{2+}] [\Sigma \text{H}_2\text{S}]$		E3
$R_4 = -k_4 [\text{Fe}^{2+}]$		E4

*Conversion factor of organic matter from wt% to mM is $\frac{1-\phi}{\phi} \frac{\rho_d}{M_C} \frac{1}{100\%}$. ρ_d is the dry bulk density (2.6 g cm⁻³), and M_C = molar weight of carbon (12 g mol⁻¹).

** Adsorption reaction after Wang and Van Capellen (1996), $\equiv \text{S} - \text{H}^0$ represents a hydrated surface site.

Table S2: Final parameters in the model and boundary conditions.

	Symbol	Unit	Value
Parameters			
Porosity	ϕ	-	0.7
Sedimentation rate	ω	cm yr ⁻¹	0.16
Sediment thickness		cm	400
C _{org}	G ₀	wt%	0.12
1 st order deg. coeff. C _{org}	k_1	yr ⁻¹	1.0E-6
Rate constant of R2	k_2	yr ⁻¹	0.4
Rate constant of R3	k_3	mM ⁻¹ yr ⁻¹	4.0
Rate constant of R4	k_4	yr ⁻¹	1.0E-5
Fractionation factor for R1	α_1	-	0.997
Fractionation factor for R2	α_2	-	1.000
Fractionation factor for R3	α_3	-	0.998
Fractionation factor for R4	α_4	-	1.004
$\delta^{56}\text{Fe}_{\text{Fe}(\text{OH})_3}$			0.00
Boundary condition			
Upper boundary	z ₀	cm	70
Concentration of H ₂ S at z ₀	-	μM	527
Concentration of Fe _{diss} at z ₀	-	μM	0.01
$\delta^{56}\text{Fe}_{\text{diss}}$ at z ₀	-	-	0.00
Lower boundary	z ₁	cm	470
Concentration of H ₂ S at z ₁	-	μM	0
Concentration of Fe _{diss} at z ₁	-	μM	450
$\delta^{56}\text{Fe}_{\text{diss}}$ at z ₁	-	-	0.00

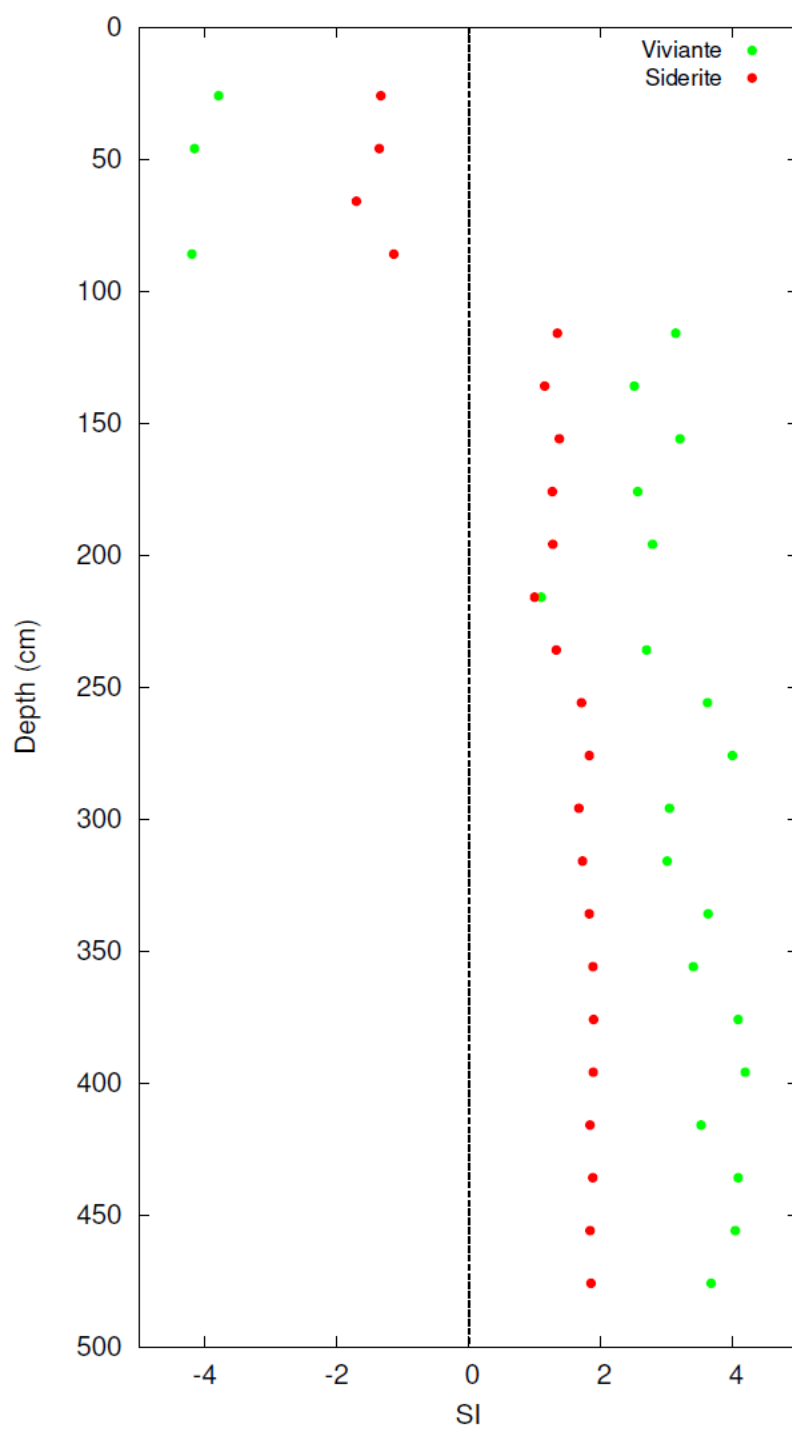


Figure S1: Saturation indices for vivianite and siderite as calculated with PHREEQC for Site HE443/010.

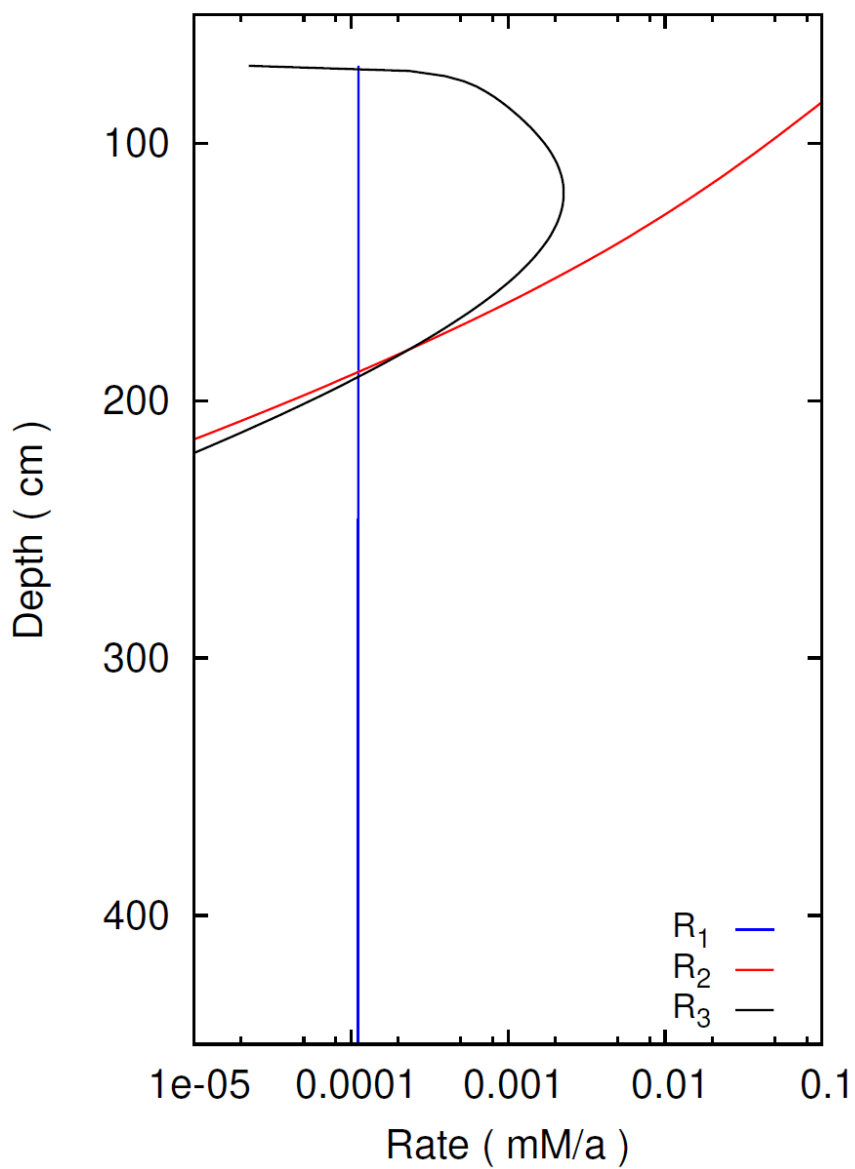


Figure S2: Reaction rates for R_1 , R_2 , and R_3 over depth as determined by fitting the model to the Fe_{diss} , H_2S and $\delta^{56}\text{Fe}_{\text{diss}}$ profiles with $k_2 = 0.4$, $k_3 = 4$, $\alpha_1 = 0.997$, $\alpha_2 = 1$, and $\alpha_3 = 0.998$.