

Boundary	Condition		
$z = 0$	Known concentration	(1)	$SO_4(0) = SO_{40}$
$z = z_{\text{bio}}$	Continuity	(2)	$SO_4(z_{\text{bio}}^-) = SO_4(z_{\text{bio}}^+)$
	Flux	(3)	$-(D_{SO_4,0} + D_{\text{bio}}) \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{\text{bio}}^-} = -D_{SO_4,0} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{\text{bio}}^+}$
$z = z_{\text{ox}}$	Continuity	(4)	$SO_4(z_{\text{ox}}^-) = SO_4(z_{\text{ox}}^+)$
	Flux	(5)	$-D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{\text{ox}}^-} + \gamma_{H_2S} \cdot F_{H_2S}(z_{\text{ox}}) = -D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{\text{ox}}^+}$
	where		$F_{H_2S}(z_{\text{ox}}) = \frac{1-\phi}{\phi} \cdot (1 - \gamma_{FeS}) \cdot \left(\int_{z_{NO_3}}^{SO_4} \sum_i SO_4 C \cdot k_i \cdot POC_i \, dz + \gamma_{CH_4} \cdot \int_{z_{SO_4}}^{z_{\text{max}}} \sum_i MC \cdot k_i \cdot POC_i \, dz \right)$
$z = z_{NO_3}$	Continuity	(6)	$SO_4(z_{NO_3}^-) = SO_4(z_{NO_3}^+)$
	Flux	(7)	$-D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{NO_3}^-} = -D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{NO_3}^+}$
$z = z_{SO_4}$	SO_4 consumption	(8)	IF ($SO_4(z_{\text{max}}) > 0$)
	($z_{SO_4} = z_{\text{max}}$)	(8.1)	$\frac{\partial SO_4}{\partial z} \Big _{z_{SO_4}} = 0$
			ELSE
	($z_{SO_4} < z_{\text{max}}$)	(8.2)	$SO_4(z_{SO_4}) = 0 \quad \text{and} \quad -D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{SO_4}} = \gamma_{CH_4} \cdot F_{CH_4}(z_{SO_4})$
$\frac{\partial SO_4}{\partial z} \Big _{z_{SO_4}} = 0$			
	with		$F_{CH_4}(z_{SO_4}) = \frac{1-\phi}{\phi} \cdot \int_{z_{SO_4}}^{z_{\text{max}}} \sum_i MC \cdot k_i \cdot POC_i \, dz$
$z = 0$	Known concentration	(1)	$H_2S(0) = H_2S_0$
$z = z_{\text{bio}}$	Continuity	(2)	$H_2S(z_{\text{bio}}^-) = H_2S(z_{\text{bio}}^+)$
	Flux	(3)	$-(D_{H_2S,0} + D_{\text{bio}}) \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{\text{bio}}^-} = -D_{H_2S,0} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{\text{bio}}^+}$
$z = z_{\text{ox}}$	Continuity	(4)	$H_2S(z_{\text{ox}}^-) = H_2S(z_{\text{ox}}^+)$
	Flux	(5)	$-D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{\text{ox}}^-} - \gamma_{H_2S} F_{H_2S}(z_{\text{ox}}) = -D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{\text{ox}}^+}$
	where		$F_{H_2S}(z_{\text{ox}}) = \frac{1-\phi}{\phi} \cdot (1 - \gamma_{FeS}) \cdot \left(\int_{z_{NO_3}}^{SO_4} \sum_i SO_4 C \cdot k_i \cdot POC_i \, dz + \gamma_{CH_4} \cdot \int_{z_{SO_4}}^{z_{\text{max}}} \sum_i MC \cdot k_i \cdot POC_i \, dz \right)$
$z = z_{NO_3}$	Continuity	(6)	$H_2S(z_{NO_3}^-) = H_2S(z_{NO_3}^+)$
	Flux	(7)	$-D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{NO_3}^-} = -D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{NO_3}^+}$
$z = z_{SO_4}$	Continuity	(8)	$H_2S(z_{SO_4}^-) = H_2S(z_{SO_4}^+)$
	Flux (with AOM)	(9)	$-D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{SO_4}^-} + \gamma_{CH_4} \cdot F_{CH_4}(z_{SO_4}) = -D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{SO_4}^+}$
	where		$F_{CH_4}(z_{SO_4}) = \frac{1-\phi}{\phi} \cdot \int_{z_{SO_4}}^{z_{\text{max}}} \sum_i MC \cdot k_i \cdot POC_i \, dz$
$z = z_{\text{max}}$	Zero H_2S flux	(10)	$\frac{\partial H_2S}{\partial z} \Big _{z_{\text{max}}} = 0$