

| Boundary | Condition | | |
|-----------------------|--|-------|---|
| $z = 0$ | Known concentration | (1) | $\text{NO}_3(0) = \text{NO}_{30}$ |
| $z = z_{\text{bio}}$ | Continuity | (2) | $\text{NO}_3(z_{\text{bio}}^-) = \text{NO}_3(z_{\text{bio}}^+)$ |
| | | (3) | $-(D_{\text{NO}_3,0} + D_{\text{bio}}) \cdot \frac{\partial \text{NO}_3}{\partial z} \Big _{z_{\text{bio}}^-} = -D_{\text{NO}_3,0} \cdot \frac{\partial \text{NO}_3}{\partial z} \Big _{z_{\text{bio}}^+}$ |
| $z = z_{\text{ox}}$ | Continuity | (4) | $\text{NO}_3(z_{\text{ox}}^-) = \text{NO}_3(z_{\text{ox}}^+)$ |
| | | (5) | $-D_{\text{NO}_3} \cdot \frac{\partial \text{NO}_3}{\partial z} \Big _{z_{\text{ox}}^-} + \gamma_{\text{NH}_4} \cdot F_{\text{NH}_4}(z_{\text{ox}}) = -D_{\text{NO}_3} \cdot \frac{\partial \text{NO}_3}{\partial z} \Big _{z_{\text{ox}}^+}$ |
| | where | | $F_{\text{NH}_4}(z_{\text{ox}}) = \frac{1}{1+K_{\text{NH}_4}} \cdot \frac{1-\phi}{\phi} \cdot \int_{z_{\text{NO}_3}}^{z_{\text{max}}} \sum_i \text{NC}_i \cdot k_i \cdot \text{POC}_i \, dz$ |
| $z = z_{\text{NO}_3}$ | NO_3 consumption | (6) | IF ($\text{NO}_3(z_{\text{max}}) > 0$) |
| | ($z_{\text{NO}_3} = z_{\text{max}}$) | (6.1) | $\frac{\partial \text{NO}_3}{\partial z} \Big _{z_{\text{NO}_3}} = 0$ |
| | | | ELSE |
| | ($z_{\text{NO}_3} < z_{\text{max}}$) | (6.2) | $\text{NO}_3(z_{\text{NO}_3}) = 0$ and $\frac{\partial \text{NO}_3}{\partial z} \Big _{z_{\text{NO}_3}} = 0$ |
| $z = 0$ | Known concentration | (1) | $\text{NH}_4(0) = \text{NH}_{40}$ |
| $z = z_{\text{bio}}$ | Continuity | (2) | $\text{NH}_4(z_{\text{bio}}^-) = \text{NH}_4(z_{\text{bio}}^+)$ |
| | | (3) | $-\frac{D_{\text{NH}_4,0} + D_{\text{bio}}}{1+K_{\text{NH}_4}} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{bio}}^-} = -\frac{D_{\text{NH}_4,0}}{1+K_{\text{NH}_4}} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{bio}}^+}$ |
| $z = z_{\text{ox}}$ | Continuity | (4) | $\text{NH}_4(z_{\text{ox}}^-) = \text{NH}_4(z_{\text{ox}}^+)$ |
| | | (5) | $-\frac{D_{\text{NH}_4}}{1+K_{\text{NH}_4}} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{ox}}^-} - \gamma_{\text{NH}_4} \cdot F_{\text{NH}_4}(z_{\text{ox}}) = -\frac{D_{\text{NH}_4}}{1+K_{\text{NH}_4}} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{ox}}^+}$ |
| | where | | $F_{\text{NH}_4}(z_{\text{ox}}) = \frac{1}{1+K_{\text{NH}_4}} \cdot \frac{1-\phi}{\phi} \cdot \int_{z_{\text{NO}_3}}^{z_{\text{max}}} \sum_i \text{NC}_i \cdot k_i \cdot \text{POC}_i \, dz$ |
| $z = z_{\text{NO}_3}$ | Continuity | (6) | $\text{NH}_4(z_{\text{NO}_3}^-) = \text{NH}_4(z_{\text{NO}_3}^+)$ |
| | Flux | (7) | $-\frac{D_{\text{NH}_4}}{1+K_{\text{NH}_4}} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{NO}_3}^-} = -\frac{D_{\text{NH}_4}}{1+K_{\text{NH}_4}} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{NO}_3}^+}$ |
| $z = z_{\text{max}}$ | Zero NH_4 flux | (8) | $\frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{max}}} = 0$ |