A.4 Numerical solution of OTIS-R model equations

The solution is similar to the solution of the OTIS model equations proposed by Runkel (1998), with small changes due to the terms added for OTIS-R.

A.4.1 Differential equations

$$\frac{\partial C}{\partial t} = -\frac{Q}{A}\frac{\partial C}{\partial x} + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right) + \frac{q_I}{A}(C_I - C) - \lambda C - \frac{k}{d}C + \alpha(C_H - C) + \rho\hat{\lambda}(C_{\text{sed}} - K_d C) \tag{A.11}$$

$$\frac{dC_H}{dt} = \alpha\frac{A}{A_H}(C - C_H) - \lambda_H C_H + \gamma + \hat{\lambda}_H(\hat{C}_H - C_H) \tag{A.12}$$

$$\frac{dC_{\text{sed}}}{dt} = \hat{\lambda}(K_d C - C_{\text{sed}}) \tag{A.13}$$

A.4.2 Steady-state equations

condition: $\frac{\partial C}{\partial t} = 0$, $\frac{dC_H}{dt} = 0$, $\frac{dC_{\text{sed}}}{dt} = 0$

Equation A.11 becomes:

$$0 = -\frac{Q}{A}\frac{\partial C}{\partial x} + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right) + \frac{q_I}{A}(C_I - C) - \lambda C - \frac{k}{d}C + \alpha(C_H - C) + \rho\hat{\lambda}(C_{\text{sed}} - K_d C) \tag{A.14}$$

Equation A.12 becomes:

$$0 = \alpha\frac{A}{A_H}(C - C_H) - \lambda_H C_H + \hat{\lambda}_H(\hat{C}_H - C_H) \tag{A.15}$$

$$0 = \alpha\frac{A}{A_H}C - \alpha\frac{A}{A_H}C_H - \lambda_H C_H + \gamma + \hat{\lambda}_H\hat{C}_H - \hat{\lambda}_H C_H$$

$$0 = \alpha\frac{A}{A_H}C + \gamma + \hat{\lambda}_H\hat{C}_H - \left(\alpha\frac{A}{A_H} + \lambda_H + \hat{\lambda}_H\right)C_H$$

$$\left(\alpha\frac{A}{A_H} + \lambda_H + \hat{\lambda}_H\right)C_H = \alpha\frac{A}{A_H}C + \gamma + \hat{\lambda}_H\hat{C}_H$$

$$C_H = \frac{\alpha\frac{A}{A_H}C + \gamma + \hat{\lambda}_H\hat{C}_H}{\alpha\frac{A}{A_H} + \lambda_H + \hat{\lambda}_H}$$

$$\boxed{C_H = \frac{\alpha AC + \gamma A_H + \hat{\lambda}_H\hat{C}_H A_H}{\alpha A + \lambda_H A_H + \hat{\lambda}_H A_H}} \tag{A.16}$$

Equation A.13 becomes:

$$0 = \hat{\lambda}(K_d C - C_{\text{sed}}) \tag{A.17}$$

$$0 = \hat{\lambda}K_d C - \hat{\lambda}C_{\text{sed}}$$

$$\boxed{C_{\text{sed}} = K_d C} \tag{A.18}$$

A.4.3 Numerical solution - Time variable

Finite differences

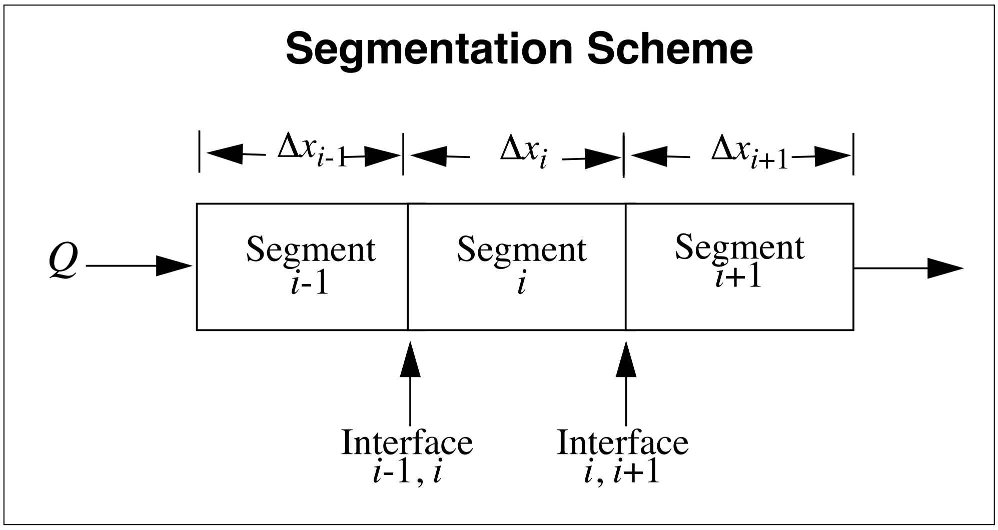

Figure A.1: Segmentation scheme for the finite differences method. Image from (Runkel, 1998, Fig. 4)

Using the finite differences approximation illustrated in Figure A.1 Runkel (1998), Equation A.11 becomes:

$$\frac{dC}{dt} = -\left(\frac{Q}{A}\right)_i \left(\frac{C_{i+1} - C_{i-1}}{2\Delta x}\right) + \frac{1}{A_i}\left(\frac{(AD)_{i,i+1}(C_{i+1} - C_i) - (AD)_{i-1,i}(C_i - C_{i-1})}{\Delta x^2}\right)$$
$$+ \frac{q_I}{A_i}(C_I - C_i) - \lambda C_i - \frac{k}{d_i}C_i + \alpha(C_H - C_i) + \rho\hat{\lambda}(C_{\text{sed}} - K_d C_i) \quad \text{(A.19)}$$

The Crank-Nicolson method for the main channel concentration

Applying the Crank-Nicolson method, the time derivative of C becomes:

$$\frac{dC}{dt} = \frac{C_i^{j+1} - C_i^j}{\Delta t} \quad \text{(A.20)}$$

where j is the current time and $j + 1$ a future time. Equation A.19 then becomes:

$$\frac{C_i^{j+1} - C_i^j}{\Delta t} = \frac{G[C, C_H, C_{\text{sed}}]^{j+1} + G[C, C_H, C_{\text{sed}}]^j}{2} \quad \text{(A.21)}$$

where:

$$G[C, C_H, C_{\text{sed}}] = -\left(\frac{Q}{A}\right)_i \left(\frac{C_{i+1} - C_{i-1}}{2\Delta x}\right) + \frac{1}{A_i}\left(\frac{(AD)_{i,i+1}(C_{i+1} - C_i) - (AD)_{i-1,i}(C_i - C_{i-1})}{\Delta x^2}\right)$$
$$+ \frac{q_I}{A_i}(C_I - C_i) - \lambda C_i - \frac{k}{d_i}C_i + \alpha(C_H - C_i) + \rho\hat{\lambda}(C_{\text{sed}} - K_d C_i)$$

then:

$$\begin{aligned}\frac{C_i^{j+1}-C_i^j}{\Delta t} =& \frac{1}{2}\Bigg[-\left(\frac{Q}{A}\right)_i^{j+1}\left(\frac{C_{i+1}^{j+1}-C_{i-1}^{j+1}}{2\Delta x}\right)\\ &+\frac{1}{A_i^{j+1}}\left(\frac{(AD)_{i,i+1}^{j+1}(C_{i+1}^{j+1}-C_i^{j+1})-(AD)_{i-1,i}^{j+1}(C_i^{j+1}-C_{i-1}^{j+1})}{\Delta x^2}\right)\\ &+\frac{q_I^{j+1}}{A_i^{j+1}}(C_I^{j+1}-C_i^{j+1})-\lambda C_i^{j+1}-\frac{k}{d_i^{j+1}}C_i^{j+1}+\alpha(C_H^{j+1}-C_i^{j+1})\\ &+\rho\hat{\lambda}(C_{\text{sed}}^{j+1}-K_d C_i^{j+1})+G[C,C_H,C_{\text{sed}}]^j\Bigg]\end{aligned} \tag{A.22}$$

Shifting all known quantities in Equation A.22 on the right side and all unknown quantities on the left side leads to:

$$\begin{aligned}C_i^{j+1}-\frac{\Delta t}{2}\Bigg[&-\left(\frac{Q}{A}\right)_i^{j+1}\left(\frac{C_{i+1}^{j+1}-C_{i-1}^{j+1}}{2\Delta x}\right)\\ &+\frac{1}{A_i^{j+1}}\left(\frac{(AD)_{i,i+1}^{j+1}(C_{i+1}^{j+1}-C_i^{j+1})-(AD)_{i-1,i}^{j+1}(C_i^{j+1}-C_{i-1}^{j+1})}{\Delta x^2}\right)\\ &-\frac{q_I^{j+1}}{A_i^{j+1}}C_i^{j+1}-\lambda C_i^{j+1}-\frac{k}{d_i^{j+1}}C_i^{j+1}-\alpha C_i^{j+1}-\rho\hat{\lambda}K_d C_i^{j+1}\Bigg]\\ &=C_i^j+\frac{\Delta t}{2}\left[\frac{q_I^{j+1}}{A_i^{j+1}}C_I^{j+1}+\alpha C_H^{j+1}+\rho\hat{\lambda}C_{\text{sed}}^{j+1}+G[C,C_H,C_{\text{sed}}]^j\right]\end{aligned}$$

$$\begin{aligned}\left(1+\frac{\Delta t}{2}\left[\frac{q_I^{j+1}}{A_i^{j+1}}+\lambda+\frac{k}{d_i^{j+1}}+\alpha+\rho\hat{\lambda}K_d\right]\right)C_i^{j+1}-\frac{\Delta t}{2}\Bigg[&-\left(\frac{Q}{A}\right)_i^{j+1}\left(\frac{C_{i+1}^{j+1}-C_{i-1}^{j+1}}{2\Delta x}\right)\\ +\frac{1}{A_i^{j+1}}\left(\frac{(AD)_{i,i+1}^{j+1}(C_{i+1}^{j+1}-C_i^{j+1})-(AD)_{i-1,i}^{j+1}(C_i^{j+1}-C_{i-1}^{j+1})}{\Delta x^2}\right)\Bigg]&\\ =C_i^j+\frac{\Delta t}{2}\left[\frac{q_I^{j+1}}{A_i^{j+1}}C_I^{j+1}+\alpha C_H^{j+1}+\rho\hat{\lambda}C_{\text{sed}}^{j+1}+G[C,C_H,C_{\text{sed}}]^j\right]&\end{aligned} \tag{A.23}$$

Grouping Equation A.23 leads to:

$$\boxed{E_i C_{i-1}^{j+1}+F_i C_i^{j+1}+G_i C_{i+1}^{j+1}=R_i} \tag{A.24}$$

where:

$$\begin{aligned}E_i C_{i-1}^{j+1}&=-\frac{\Delta t}{2}\left[-\left(\frac{Q}{A}\right)_i^{j+1}\left(\frac{-C_{i-1}^{j+1}}{2\Delta x}\right)+\frac{1}{A_i^{j+1}}\left(\frac{-(AD)_{i-1,i}^{j+1}(-C_{i-1}^{j+1})}{\Delta x^2}\right)\right]\\ E_i C_{i-1}^{j+1}&=-\frac{\Delta t}{2A_i^{j+1}\Delta x}\left(\frac{Q_i^{j+1}C_i^{j+1}}{2}+\frac{(AD)_{i-1,i}^{j+1}C_{i-1}^{j+1}}{\Delta x}\right)\\ &\boxed{E_i=-\frac{\Delta t}{2A_i^{j+1}\Delta x}\left(\frac{Q_i^{j+1}}{2}+\frac{(AD)_{i-1,i}^{j+1}}{\Delta x}\right)}\end{aligned} \tag{A.25}$$

$$
\begin{aligned}
F_i C_i^{j+1} =& \left(1 + \frac{\Delta t}{2}\left[\frac{q_I^{j+1}}{A_i^{j+1}} + \lambda + \frac{k}{d_i^{j+1}} + \alpha + \rho\hat{\lambda}K_d\right]\right) C_i^{j+1} \\
&- \frac{\Delta t}{2}\left[\frac{1}{A_i^{j+1}} \frac{(AD)_{i,i+1}^{j+1}(-C_i^{j+1}) - (AD)_{i-1,i}^{j+1} C_i^{j+1}}{\Delta x^2}\right] \\
F_i C_i^{j+1} =& \left(1 + \frac{\Delta t}{2}\left[\frac{q_I^{j+1}}{A_i^{j+1}} + \lambda + \frac{k}{d_i^{j+1}} + \alpha + \rho\hat{\lambda}K_d\right]\right) C_i^{j+1} \\
&+ \frac{\Delta t}{2}\left[\frac{(AD)_{i,i+1}^{j+1} + (AD)_{i-1,i}^{j+1}}{A_i^{j+1}\Delta x^2}\right] C_i^{j+1} \\
F_i =& 1 + \frac{\Delta t}{2}\left(\frac{q_I^{j+1}}{A_i^{j+1}} + \lambda + \frac{k}{d_i^{j+1}} + \alpha + \rho\hat{\lambda}K_d + \frac{(AD)_{i,i+1}^{j+1} + (AD)_{i-1,i}^{j+1}}{A_i^{j+1}\Delta x^2}\right)
\end{aligned} \tag{A.26}
$$

$$
\begin{aligned}
G_i C_{i+1}^{j+1} =& -\frac{\Delta t}{2}\left(-\left(\frac{Q}{A}\right)_i^{j+1} \frac{C_{i+1}^{j+1}}{2\Delta x} + \frac{1}{A_i^{j+1}} \frac{(AD)_{i,i+1}^{j+1} C_{i+1}^{j+1}}{\Delta x^2}\right) \\
&\boxed{G_i = \frac{\Delta t}{2A_i^{j+1}\Delta x}\left(\frac{Q_i^{j+1}}{2} - \frac{(AD)_{i,i+1}^{j+1}}{\Delta x}\right)}
\end{aligned} \tag{A.27}
$$

$$
R_i = C_i^j + \frac{\Delta t}{2}\left(\frac{q_I^{j+1}}{A_i^{j+1}} C_I^{j+1} + \alpha C_H^{j+1} + \rho\hat{\lambda} C_{\mathrm{sed}}^{j+1} + G[C, C_H, C_{\mathrm{sed}}]^j\right) \tag{A.28}
$$

The Crank-Nicolson method for the hyporheic zone and streamed sediments

Applying the Crank-Nicolson method to Equation A.12 leads to:

$$
\begin{aligned}
\frac{C_H^{j+1} - C_H^j}{\Delta t} =& \frac{\left(\alpha \frac{A}{A_H}(C - C_H) - \lambda_H C_H + \gamma + \hat{\lambda}(\hat{C}_H - C_H)\right)^{j+1}}{2} \\
&+ \frac{\left(\alpha \frac{A}{A_H}(C - C_H) - \lambda_H C_H + \gamma + \hat{\lambda}(\hat{C}_H - C_H)\right)^{j}}{2}
\end{aligned} \tag{A.29}
$$

Solving Equation A.29 for C_H^{j+1} leads to:

$$
\begin{aligned}
C_H^{j+1} - C_H^j =& \frac{\Delta t}{2}\Bigg(\alpha \frac{A}{A_H} C^{j+1} - \alpha \frac{A}{A_H} C_H^{j+1} - \lambda_H C_H^{j+1} + \gamma \\
&+ \hat{\lambda}_H \hat{C}_H - \hat{\lambda}_H C_H^{j+1} + \alpha \frac{A}{A_H} C^j - \alpha \frac{A}{A_H} C_H^j \\
&- \lambda_H C_H^j + \gamma + \hat{\lambda}_H \hat{C}_H - \hat{\lambda}_H C_H^j \Bigg) \\
0 =& \frac{\Delta t}{2}\alpha \frac{A}{A_H} C^{j+1} - \frac{\Delta t}{2}\alpha \frac{A}{A_H} C_H^{j+1} - \frac{\Delta t}{2}\lambda_H C_H^{j+1} \\
&+ \frac{\Delta t}{2}\gamma + \frac{\Delta t}{2}\hat{\lambda}_H \hat{C}_H - \frac{\Delta t}{2}\hat{\lambda}_H C_H^{j+1} \\
&+ \frac{\Delta t}{2}\alpha \frac{A}{A_H} C^j - \frac{\Delta t}{2}\alpha \frac{A}{A_H} C_H^j - \frac{\Delta t}{2}\lambda_H C_H^j \\
&+ \frac{\Delta t}{2}\gamma + \frac{\Delta t}{2}\hat{\lambda}_H \hat{C}_H - \frac{\Delta t}{2}\hat{\lambda}_H C_H^j \\
0 =& \frac{\Delta t}{2}\alpha \frac{A}{A_H} C^{j+1} + \frac{\Delta t}{2}\gamma + \frac{\Delta t}{2}\gamma + \frac{\Delta t}{2}\hat{\lambda}_H \hat{C}_H \\
&+ \frac{\Delta t}{2}\hat{\lambda}_H \hat{C}_H + \frac{\Delta t}{2}\alpha \frac{A}{A_H} C^j \\
&+ \left(-\frac{\Delta t}{2}\alpha \frac{A}{A_H} - \frac{\Delta t}{2}\lambda_H - \frac{\Delta t}{2}\hat{\lambda}_H + 1\right) C_H^j \\
&- \left(\frac{\Delta t}{2}\alpha \frac{A}{A_H} + \frac{\Delta t}{2}\lambda_H + \frac{\Delta t}{2}\hat{\lambda}_H + 1\right) C_H^{j+1} \\
\left(\Delta t \alpha \frac{A}{A_H} + \Delta t \lambda_H + \Delta t \hat{\lambda}_H + 2\right) C_H^{j+1} =& \Delta t \alpha \frac{A}{A_H} C^{j+1} + 2\Delta t \gamma + 2\Delta t \hat{\lambda}_H \hat{C}_H + \Delta t \alpha \frac{A}{A_H} C^j \\
&+ 2\left(2 - \Delta t \alpha \frac{A}{A_H} - \Delta t \lambda_H - \Delta t \hat{\lambda}_H\right) C_H^j
\end{aligned}
$$

$$
C_H^{j+1} = \frac{\left(2 - \Delta t \alpha \frac{A}{A_H} - \Delta t \lambda_H - \Delta t \hat{\lambda}_H\right) C_H^j + \Delta t \alpha \frac{A}{A_H} C^{j+1} + \Delta t \alpha \frac{A}{A_H} C^j + 2\Delta t \hat{\lambda}_H \hat{C}_H + 2\Delta t \gamma}{2 + \Delta t \alpha \frac{A}{A_H} + \Delta t \lambda_H + \Delta t \hat{\lambda}_H} \tag{A.30}
$$

With $\mathrm{GAM} = \frac{\alpha \Delta t A}{A_H}$, Equation A.30 becomes:

$$
\boxed{C_H^{j+1} = \frac{\left(2 - \mathrm{GAM}^j - \Delta t \lambda_H - \Delta t \hat{\lambda}_H\right) C_H^j + \mathrm{GAM}^{j+1} C^{j+1} + \mathrm{GAM}^j C^j + 2\Delta t \hat{\lambda}_H \hat{C}_H + 2\Delta t \gamma}{2 + \mathrm{GAM}^{j+1} + \Delta t \lambda_H + \Delta t \hat{\lambda}_H}} \tag{A.31}
$$

Applying the Crank-Nicolson method to Equation A.13 leads to:

$$
\begin{aligned}
\frac{C_{\mathrm{sed}}^{j+1} - C_{\mathrm{sed}}^j}{\Delta t} =& \frac{\left(\hat{\lambda}(K_d C - C_{\mathrm{sed}})\right)^{j+1} \left(\hat{\lambda}(K_d C - C_{\mathrm{sed}})\right)^j}{2} \\
&\boxed{C_{\mathrm{sed}}^{j+1} = \frac{(2 - \Delta t \hat{\lambda}) C_{\mathrm{sed}} + \Delta t \hat{\lambda} K_d (C^j + C^{j+1})}{2 + \Delta t \hat{\lambda}}}
\end{aligned} \tag{A.32}
$$

Decoupling the main channel, hyporheic zone and streambed sediment equations

Substituting Equation A.31 and Equation A.30 into Equation A.28:

$$
\begin{aligned}
R_i' =& C_i^j + \frac{\Delta t}{2}\left[\frac{q_I^{j+1}}{A_i^{j+1}}C_I^{j+1}\right. \\
&+ \alpha\frac{\left(2-\mathrm{GAM}^j-\Delta t\lambda_H-\Delta t\hat{\lambda}_H\right)C_H^j+\mathrm{GAM}^{j+1}C^{j+1}+\mathrm{GAM}^jC^j+2\Delta t\hat{\lambda}_H\hat{C}_H+2\Delta t\gamma}{2+\mathrm{GAM}^{j+1}+\Delta t\lambda_H+\Delta t\hat{\lambda}_H} \\
&\left.+ \rho\hat{\lambda}\frac{(2-\Delta t\hat{\lambda})C_{\mathrm{sed}^j}+\Delta t\hat{\lambda}K_d(C^j+C^{j+1})}{2+\Delta t\hat{\lambda}} + G[C,C_H,C_{\mathrm{sed}}]^j\right]
\end{aligned}
\tag{A.33}
$$

Moving the terms containing C_i^{j+1} in Equation A.33 to Equation A.26, leads to the new F_i' and R_i'':

$$
\begin{aligned}
F_i' =& 1+\frac{\Delta t}{2}\left(\frac{q_I^{j+1}}{A_i^{j+1}}+\lambda+\frac{k}{d_i^{j+1}}+\alpha+\rho\hat{\lambda}K_d+\frac{(AD)_{i,i+1}^{j+1}+(AD)_{i-1,i}^{j+1}}{A_i^{j+1}\Delta x^2}\right) \\
&-\alpha\frac{\Delta t}{2}\left(\frac{\mathrm{GAM}^{j+1}}{2+\mathrm{GAM}^{j+1}+\Delta t\lambda_H+\Delta t\hat{\lambda}_H}\right)-\frac{\Delta t}{2}\rho\hat{\lambda}\left(\frac{\Delta t\hat{\lambda}K_d}{2+\Delta t\hat{\lambda}}\right)
\end{aligned}
$$

$$
\boxed{
\begin{aligned}
F_i' =& 1+\frac{\Delta t}{2}\left[\frac{q_I^{j+1}}{A_i^{j+1}}+\lambda+\frac{k}{d_i^{j+1}}+\alpha\left(1-\frac{\mathrm{GAM}^{j+1}}{2+\mathrm{GAM}^{j+1}+\Delta t\lambda_H+\Delta t\hat{\lambda}_H}\right)\right. \\
&\left.+\rho\hat{\lambda}K_d\left(1-\frac{\Delta t\hat{\lambda}}{2+\Delta t\hat{\lambda}}\right)+\frac{(AD)_{i,i+1}^{j+1}+(AD)_{i-1,i}^{j+1}}{A_i^{j+1}\Delta x^2}\right]
\end{aligned}
}
\tag{A.34}
$$

$$
\boxed{
\begin{aligned}
R_i'' =& C_i^j + \frac{\Delta t}{2}\left[\frac{q_I^{j+1}}{A_i^{j+1}}C_I^{j+1}\right. \\
&+ \alpha\frac{\left(2-\mathrm{GAM}^j-\Delta t\lambda_H-\Delta t\hat{\lambda}_H\right)C_H^j+\mathrm{GAM}^jC^j+2\Delta t\hat{\lambda}_H\hat{C}_H+2\Delta t\gamma}{2+\mathrm{GAM}^{j+1}+\Delta t\lambda_H+\Delta t\hat{\lambda}_H} \\
&\left.+ \rho\hat{\lambda}\frac{(2-\Delta t\hat{\lambda})C_{\mathrm{sed}^j}+\Delta t\hat{\lambda}K_dC^j}{2+\Delta t\hat{\lambda}} + G[C,C_H,C_{\mathrm{sed}}]^j\right]
\end{aligned}
}
\tag{A.35}
$$

A.4.4 Numerical solution - Steady-state

Finite differences

Using the finite differences approximation shown above (Figure A.1), Equation A.14 becomes:

$$
\begin{aligned}
0 =& -\left(\frac{Q}{A}\right)_i\left(\frac{C_{i+1}-C_{i-1}}{2\Delta x}\right)+\frac{1}{A_i}\left(\frac{(AD)_{i,i+1}(C_{i+1}-C_i)-(AD)_{i-1,i}(C_i-C_{i-1})}{\Delta x^2}\right) \\
&+\frac{q_I}{A_i}(C_I-C_i)-\lambda C_i-\frac{k}{d_i}C_i+\alpha(C_H-C_i)+\rho\hat{\lambda}(C_{\mathrm{sed}}-K_dC_i)
\end{aligned}
\tag{A.36}
$$

Substituting Equation A.16 and Equation A.18 into Equation A.36 leads to:

$$
\begin{aligned}
0 =& -\left(\frac{Q}{A}\right)_i \left(\frac{C_{i+1}-C_{i-1}}{2\Delta x}\right) + \frac{1}{A_i}\left(\frac{(AD)_{i,i+1}(C_{i+1}-C_i)-(AD)_{i-1,i}(C_i-C_{i-1})}{\Delta x^2}\right) \\
&+ \frac{q_I}{A_i}(C_I - C_i) - \lambda C_i - \frac{k}{d_i}C_i + \alpha\left(\frac{\alpha A_i C_i + \gamma A_H + \hat{\lambda}_H \hat{C}_H A_H}{\alpha A_i + \lambda_H A_H + \hat{\lambda}_H A_H} - C_i\right) \\
&+ \rho\hat{\lambda}(K_d C_i - K_d C_i) \\
0 =& -\left(\frac{Q}{A}\right)_i \left(\frac{C_{i+1}-C_{i-1}}{2\Delta x}\right) + \frac{1}{A_i}\left(\frac{(AD)_{i,i+1}(C_{i+1}-C_i)-(AD)_{i-1,i}(C_i-C_{i-1})}{\Delta x^2}\right) \\
&+ \frac{q_I}{A_i}(C_I - C_i) - \lambda C_i - \frac{k}{d_i}C_i \\
&+ \frac{\alpha^2 A_i C_i + \alpha\gamma A_H + \alpha\hat{\lambda}_H \hat{C}_H A_H - \alpha^2 A_i C_i - \alpha\lambda_H A_H C_i - \alpha\hat{\lambda}_H A_H C_i}{\alpha A_i + \lambda A_H + \hat{\lambda}_H A_H} \\
0 =& -\left(\frac{Q}{A}\right)_i \left(\frac{C_{i+1}-C_{i-1}}{2\Delta x}\right) + \frac{1}{A_i}\left(\frac{(AD)_{i,i+1}(C_{i+1}-C_i)-(AD)_{i-1,i}(C_i-C_{i-1})}{\Delta x^2}\right) \\
&+ \frac{q_I}{A_i}(C_I - C_i) - \lambda C_i - \frac{k}{d_i}C_i + \frac{\alpha A_H(\gamma + \hat{\lambda}_H \hat{C}_H - \lambda_H C_i - \hat{\lambda}_H C_i)}{\alpha A_i + \lambda A_H + \hat{\lambda}_H A_H}
\end{aligned} \tag{A.37}
$$

Rearrangement of Equation A.37 yields:

$$
\boxed{E_i C_{i-1}^{j+1} + F_i C_i^{j+1} + G_i C_{i+1}^{j+1} = R_i} \tag{A.38}
$$

where:

$$
\begin{aligned}
E_i C_{i-1} =& \left(\frac{Q}{A}\right)_i \left(\frac{-C_{i-1}}{2\Delta x}\right) - \frac{1}{A_i}\left(\frac{-(AD)_{i-1,i}(-C_{i-1})}{\Delta x^2}\right) \\
&\boxed{E_i = -\frac{1}{A_i \Delta x}\left(\frac{Q_i}{2} + \frac{(AD)_{i-1,i}}{\Delta x}\right)}
\end{aligned} \tag{A.39}
$$

$$
\begin{aligned}
F_i C_i =& -\frac{1}{A_i}\left(\frac{(AD)_{i,i+1}(-C_i) - (AD)_{i-1,i}C_i}{\Delta x^2}\right) + \frac{q_I}{A_i} + \lambda C_i + \frac{k}{d_i}C_i \\
&- \frac{\alpha A_H - \lambda_H C_i - \hat{\lambda}_H C_i}{\alpha A_i + \lambda A_H + \hat{\lambda}_H A_H} \\
&\boxed{F_i = \frac{(AD)_{i,i+1} + (AD)_{i-1,i}}{A_i \Delta x^2} + \frac{q_I}{A_i} + \lambda + \frac{k}{d_i} + \alpha A_H \frac{\lambda_H + \hat{\lambda}_H}{\alpha A_i + \lambda A_H + \hat{\lambda}_H A_H}}
\end{aligned} \tag{A.40}
$$

$$
\begin{aligned}
G_i C_{i+1} =& \left(\frac{Q}{A}\right)_i \frac{C_{i+1}}{2\Delta x} - \frac{1}{A_i}\left(\frac{(AD)_{i,i+1}C_{i+1}}{\Delta x^2}\right) \\
&\boxed{G_i = \frac{1}{A_i \Delta x}\left(\frac{Q_i}{2} - \frac{(AD)_{i,i+1}}{\Delta x}\right)}
\end{aligned} \tag{A.41}
$$

$$
\boxed{R_i = \frac{q_I}{A_i}C_I + \frac{\alpha A_H(\gamma + \hat{\lambda}_H \hat{C}_H)}{\alpha A_i + \lambda_H A_H + \hat{\lambda}_H A_H}} \tag{A.42}
$$

A.4.5 Solving the numerical equations

Equation A.24 and Equation A.38 can be solved as:

$$\begin{bmatrix} F_1^{(\prime)} & G_1 & & & \\ E_2 & F_2^{(\prime)} & G_2 & & \\ & & ... & & \\ & & E_{N-1} & F_{N-1}^{(\prime)} & G_{N-1} \\ & & & E_N & F_N^{(\prime)} \end{bmatrix} \begin{bmatrix} C_1^{j+1} \\ C_2^{j+1} \\ ... \\ C_{N-1}^{j+1} \\ C_N^{j+1} \end{bmatrix} = \begin{bmatrix} R_1^{(\prime\prime)} \\ R_2^{(\prime\prime)} \\ ... \\ R_{N-1}^{(\prime\prime)} \\ R_N^{(\prime\prime)} \end{bmatrix} \tag{A.43}$$

where N is the number of segments.