

# 1 Numerical solution of OTIS-R model equations

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

## 1.1 Differential equations

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

$$\frac{dC_H}{dt} = \alpha \frac{A}{A_H} (C - C_H) - \lambda_H C_H + \gamma + \hat{\lambda}_H (\hat{C}_H - C_H) \quad (2)$$

$$\frac{dC_{\text{sed}}}{dt} = \hat{\lambda} (K_d C - C_{\text{sed}}) \quad (3)$$

## 1.2 Steady-state equations

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

Equation 1 becomes:

$$0 = -\frac{Q}{A} \frac{\partial C}{\partial x} + \frac{1}{A} \frac{\partial}{\partial x} \left( AD \frac{\partial C}{\partial x} \right) + \frac{q_I}{A} (C_I - C) - \lambda C - \frac{k}{d} C + \alpha (C_H - C) + \rho \hat{\lambda} (C_{\text{sed}} - K_d C) \quad (4)$$

Equation 2 becomes:

$$\begin{aligned} 0 &= \alpha \frac{A}{A_H} (C - C_H) - \lambda_H C_H + \hat{\lambda}_H (\hat{C}_H - C_H) \\ 0 &= \alpha \frac{A}{A_H} C - \alpha \frac{A}{A_H} C_H - \lambda_H C_H + \gamma + \hat{\lambda}_H \hat{C}_H - \hat{\lambda}_H C_H \\ 0 &= \alpha \frac{A}{A_H} C + \gamma + \hat{\lambda}_H \hat{C}_H - \left( \alpha \frac{A}{A_H} + \lambda_H + \hat{\lambda}_H \right) C_H \\ \left( \alpha \frac{A}{A_H} + \lambda_H + \hat{\lambda}_H \right) C_H &= \alpha \frac{A}{A_H} C + \gamma + \hat{\lambda}_H \hat{C}_H \\ C_H &= \frac{\alpha \frac{A}{A_H} C + \gamma + \hat{\lambda}_H \hat{C}_H}{\alpha \frac{A}{A_H} + \lambda_H + \hat{\lambda}_H} \\ \boxed{C_H} &= \frac{\alpha AC + \gamma A_H + \hat{\lambda}_H \hat{C}_H A_H}{\alpha A + \lambda_H A_H + \hat{\lambda}_H A_H} \end{aligned} \quad (5) \quad (6)$$

Equation 3 becomes:

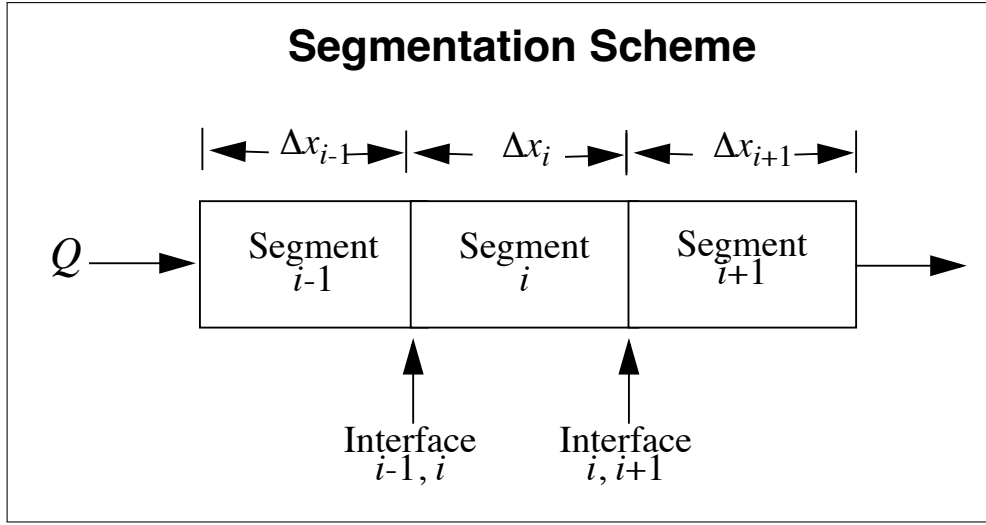
$$0 = \hat{\lambda}(K_d C - C_{\text{sed}}) \quad (7)$$

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

$$\boxed{C_{\text{sed}} = K_d C} \quad (8)$$

### 1.3 Numerical solution - Time variable

#### Finite differences



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

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

$$\begin{aligned} \frac{dC}{dt} = & - \left( \frac{Q}{A} \right)_i \left( \frac{C_{i+1} - C_{i-1}}{2\Delta x} \right) + \frac{1}{A_i} \left( \frac{(AD)_{i,i+1}(C_{i+1} - C_i) - (AD)_{i-1,i}(C_i - C_{i-1})}{\Delta x^2} \right) \\ & + \frac{q_I}{A_i} (C_I - C_i) - \lambda C_i - \frac{k}{d_i} C_i + \alpha (C_H - C_i) + \rho \hat{\lambda} (C_{\text{sed}} - K_d C_i) \end{aligned} \quad (9)$$

#### The Crank-Nicolson method for the main channel concentration

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

$$\frac{dC}{dt} = \frac{C_i^{j+1} - C_i^j}{\Delta t} \quad (10)$$

where  $j$  is the current time and  $j + 1$  a future time. Equation 9 then becomes:

$$\frac{C_i^{j+1} - C_i^j}{\Delta t} = \frac{G[C, C_H, C_{\text{sed}}]^{j+1} + G[C, C_H, C_{\text{sed}}]^j}{2} \quad (11)$$

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:

$$\frac{C_i^{j+1} - C_i^j}{\Delta t} = \frac{1}{2} \left[ - \left( \frac{Q}{A} \right)_i^{j+1} \left( \frac{C_{i+1}^{j+1} - C_{i-1}^{j+1}}{2\Delta x} \right) \right. \\ + \frac{1}{A_i^{j+1}} \left( \frac{(AD)_{i,i+1}^{j+1}(C_{i+1}^{j+1} - C_i^{j+1}) - (AD)_{i-1,i}^{j+1}(C_i^{j+1} - C_{i-1}^{j+1})}{\Delta x^2} \right) \\ + \frac{q_I^{j+1}}{A_i^{j+1}}(C_I^{j+1} - C_i^{j+1}) - \lambda C_i^{j+1} - \frac{k}{d_i^{j+1}}C_i^{j+1} + \alpha(C_H^{j+1} - C_i^{j+1}) \\ \left. + \rho\hat{\lambda}(C_{\text{sed}}^{j+1} - K_d C_i^{j+1}) + G[C, C_H, C_{\text{sed}}]^j \right] \quad (12)$$

Shifting all known quantities in Equation 12 on the right side and all unknown quantities on the left side leads to:

$$C_i^{j+1} - \frac{\Delta t}{2} \left[ - \left( \frac{Q}{A} \right)_i^{j+1} \left( \frac{C_{i+1}^{j+1} - C_{i-1}^{j+1}}{2\Delta x} \right) \right. \\ + \frac{1}{A_i^{j+1}} \left( \frac{(AD)_{i,i+1}^{j+1}(C_{i+1}^{j+1} - C_i^{j+1}) - (AD)_{i-1,i}^{j+1}(C_i^{j+1} - C_{i-1}^{j+1})}{\Delta x^2} \right) \\ \left. - \frac{q_I^{j+1}}{A_i^{j+1}}C_i^{j+1} - \lambda C_i^{j+1} - \frac{k}{d_i^{j+1}}C_i^{j+1} - \alpha C_i^{j+1} - \rho\hat{\lambda}K_d C_i^{j+1} \right] \\ = C_i^j + \frac{\Delta t}{2} \left[ \frac{q_I^{j+1}}{A_i^{j+1}}C_I^{j+1} + \alpha C_H^{j+1} + \rho\hat{\lambda}C_{\text{sed}}^{j+1} + G[C, C_H, C_{\text{sed}}]^j \right] \\ \left( 1 + \frac{\Delta t}{2} \left[ \frac{q_I^{j+1}}{A_i^{j+1}} + \lambda + \frac{k}{d_i^{j+1}} + \alpha + \rho\hat{\lambda}K_d \right] \right) C_i^{j+1} - \frac{\Delta t}{2} \left[ - \left( \frac{Q}{A} \right)_i^{j+1} \left( \frac{C_{i+1}^{j+1} - C_{i-1}^{j+1}}{2\Delta x} \right) \right. \\ + \frac{1}{A_i^{j+1}} \left( \frac{(AD)_{i,i+1}^{j+1}(C_{i+1}^{j+1} - C_i^{j+1}) - (AD)_{i-1,i}^{j+1}(C_i^{j+1} - C_{i-1}^{j+1})}{\Delta x^2} \right) \\ \left. = C_i^j + \frac{\Delta t}{2} \left[ \frac{q_I^{j+1}}{A_i^{j+1}}C_I^{j+1} + \alpha C_H^{j+1} + \rho\hat{\lambda}C_{\text{sed}}^{j+1} + G[C, C_H, C_{\text{sed}}]^j \right] \right] \quad (13)$$

Grouping Equation 13 leads to:

$$\boxed{E_i C_{i-1}^{j+1} + F_i C_i^{j+1} + G_i C_{i+1}^{j+1} = R_i} \quad (14)$$

where:

$$\begin{aligned}
 E_i C_{i-1}^{j+1} &= -\frac{\Delta t}{2} \left[ -\left(\frac{Q}{A}\right)_i^{j+1} \left(\frac{-C_{i-1}^{j+1}}{2\Delta x}\right) + \frac{1}{A_i^{j+1}} \left(\frac{-(AD)_{i-1,i}^{j+1}(-C_{i-1}^{j+1})}{\Delta x^2}\right) \right] \\
 E_i C_{i-1}^{j+1} &= -\frac{\Delta t}{2A_i^{j+1}\Delta x} \left( \frac{Q_i^{j+1}C_{i-1}^{j+1}}{2} + \frac{(AD)_{i-1,i}^{j+1}C_{i-1}^{j+1}}{\Delta x} \right) \\
 E_i &= -\frac{\Delta t}{2A_i^{j+1}\Delta x} \left( \frac{Q_i^{j+1}}{2} + \frac{(AD)_{i-1,i}^{j+1}}{\Delta x} \right)
 \end{aligned} \tag{15}$$

$$\begin{aligned}
 F_i C_i^{j+1} &= \left( 1 + \frac{\Delta t}{2} \left[ \frac{q_I^{j+1}}{A_i^{j+1}} + \lambda + \frac{k}{d_i^{j+1}} + \alpha + \rho \hat{\lambda} K_d \right] \right) C_i^{j+1} \\
 &\quad - \frac{\Delta t}{2} \left[ \frac{1}{A_i^{j+1}} \frac{(AD)_{i,i+1}^{j+1}(-C_i^{j+1}) - (AD)_{i-1,i}^{j+1}C_i^{j+1}}{\Delta x^2} \right] \\
 F_i C_i^{j+1} &= \left( 1 + \frac{\Delta t}{2} \left[ \frac{q_I^{j+1}}{A_i^{j+1}} + \lambda + \frac{k}{d_i^{j+1}} + \alpha + \rho \hat{\lambda} K_d \right] \right) C_i^{j+1} \\
 &\quad + \frac{\Delta t}{2} \left[ \frac{(AD)_{i,i+1}^{j+1} + (AD)_{i-1,i}^{j+1}}{A_i^{j+1}\Delta x^2} \right] C_i^{j+1} \\
 F_i &= 1 + \frac{\Delta t}{2} \left( \frac{q_I^{j+1}}{A_i^{j+1}} + \lambda + \frac{k}{d_i^{j+1}} + \alpha + \rho \hat{\lambda} K_d + \frac{(AD)_{i,i+1}^{j+1} + (AD)_{i-1,i}^{j+1}}{A_i^{j+1}\Delta x^2} \right)
 \end{aligned} \tag{16}$$

$$\begin{aligned}
 G_i C_{i+1}^{j+1} &= -\frac{\Delta t}{2} \left( -\left(\frac{Q}{A}\right)_i^{j+1} \frac{C_{i+1}^{j+1}}{2\Delta x} + \frac{1}{A_i^{j+1}} \frac{(AD)_{i,i+1}^{j+1}C_{i+1}^{j+1}}{\Delta x^2} \right) \\
 G_i &= \frac{\Delta t}{2A_i^{j+1}\Delta x} \left( \frac{Q_i^{j+1}}{2} - \frac{(AD)_{i,i+1}^{j+1}}{\Delta x} \right)
 \end{aligned} \tag{17}$$

$$R_i = C_i^j + \frac{\Delta t}{2} \left( \frac{q_I^{j+1}}{A_i^{j+1}} C_I^{j+1} + \alpha C_H^{j+1} + \rho \hat{\lambda} C_{\text{sed}}^{j+1} + G[C, C_H, C_{\text{sed}}]^j \right) \tag{18}$$

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

Applying the Crank-Nicolson method to Equation 2 leads to:

$$\begin{aligned}
 \frac{C_H^{j+1} - C_H^j}{\Delta t} &= \frac{\left( \alpha \frac{A}{A_H} (C - C_H) - \lambda_H C_H + \gamma + \hat{\lambda} (\hat{C}_H - C_H) \right)^{j+1}}{2} \\
 &\quad + \frac{\left( \alpha \frac{A}{A_H} (C - C_H) - \lambda_H C_H + \gamma + \hat{\lambda} (\hat{C}_H - C_H) \right)^j}{2}
 \end{aligned} \tag{19}$$

Solving Equation 19 for  $C_H^{j+1}$  leads to:

$$\begin{aligned}
C_H^{j+1} - C_H^j &= \frac{\Delta t}{2} \left( \alpha \frac{A}{A_H} C_H^{j+1} - \alpha \frac{A}{A_H} C_H^{j+1} - \lambda_H C_H^{j+1} + \gamma \right. \\
&\quad \left. + \hat{\lambda}_H \hat{C}_H - \hat{\lambda}_H C_H^{j+1} + \alpha \frac{A}{A_H} C_H^j - \alpha \frac{A}{A_H} C_H^j \right. \\
&\quad \left. - \lambda_H C_H^j + \gamma + \hat{\lambda}_H \hat{C}_H - \hat{\lambda}_H C_H^j \right) \\
0 &= \frac{\Delta t}{2} \alpha \frac{A}{A_H} C_H^{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} \\
&\quad + \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} \\
&\quad + \frac{\Delta t}{2} \alpha \frac{A}{A_H} C_H^j - \frac{\Delta t}{2} \alpha \frac{A}{A_H} C_H^j - \frac{\Delta t}{2} \lambda_H C_H^j \\
&\quad + \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_H^{j+1} + \frac{\Delta t}{2} \gamma + \frac{\Delta t}{2} \gamma + \frac{\Delta t}{2} \hat{\lambda}_H \hat{C}_H \\
&\quad + \frac{\Delta t}{2} \hat{\lambda}_H \hat{C}_H + \frac{\Delta t}{2} \alpha \frac{A}{A_H} C_H^j \\
&\quad + \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 \\
&\quad - \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_H^{j+1} + 2 \Delta t \gamma + 2 \Delta t \hat{\lambda}_H \hat{C}_H + \Delta t \alpha \frac{A}{A_H} C_H^j \\
&\quad + 2 \left( 2 - \Delta t \alpha \frac{A}{A_H} - \Delta t \lambda_H - \Delta t \hat{\lambda}_H \right) C_H^j \\
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_H^{j+1} + \Delta t \alpha \frac{A}{A_H} C_H^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}
\end{aligned} \tag{20}$$

With  $GAM = \frac{\alpha \Delta t A}{A_H}$ , Equation 20 becomes:

$$C_H^{j+1} = \frac{\left( 2 - GAM^j - \Delta t \lambda_H - \Delta t \hat{\lambda}_H \right) C_H^j + GAM^{j+1} C_H^{j+1} + GAM^j C_H^j + 2 \Delta t \hat{\lambda}_H \hat{C}_H + 2 \Delta t \gamma}{2 + GAM^{j+1} + \Delta t \lambda_H + \Delta t \hat{\lambda}_H} \tag{21}$$

Applying the Crank-Nicolson method to Equation 3 leads to:

$$\frac{C_{\text{sed}}^{j+1} - C_{\text{sed}}^j}{\Delta t} = \frac{\left(\hat{\lambda}(K_d C - C_{\text{sed}})\right)^{j+1} \left(\hat{\lambda}(K_d C - C_{\text{sed}})\right)^j}{2}$$

$$\boxed{C_{\text{sed}}^{j+1} = \frac{(2 - \Delta t \hat{\lambda})C_{\text{sed}} + \Delta t \hat{\lambda} K_d (C^j + C^{j+1})}{2 + \Delta t \hat{\lambda}}} \quad (22)$$

### Decoupling the main channel, hyporheic zone and streambed sediment equations

Substituting Equation 21 and Equation 20 into Equation 18:

$$R'_i = C_i^j + \frac{\Delta t}{2} \left[ \frac{q_I^{j+1}}{A_i^{j+1}} C_I^{j+1} \right. \\ \left. + \alpha \frac{\left(2 - \text{GAM}^j - \Delta t \lambda_H - \Delta t \hat{\lambda}_H\right) C_H^j + \text{GAM}^{j+1} C^{j+1} + \text{GAM}^j C^j + 2\Delta t \hat{\lambda}_H \hat{C}_H + 2\Delta t \gamma}{2 + \text{GAM}^{j+1} + \Delta t \lambda_H + \Delta t \hat{\lambda}_H} \right. \\ \left. + \rho \hat{\lambda} \frac{(2 - \Delta t \hat{\lambda}) C_{\text{sed}}^j + \Delta t \hat{\lambda} K_d (C^j + C^{j+1})}{2 + \Delta t \hat{\lambda}} + G[C, C_H, C_{\text{sed}}]^j \right] \quad (23)$$

Moving the terms containing  $C_i^{j+1}$  in Equation 23 to Equation 16, leads to the new  $F'_i$  and  $R''_i$ :

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

$$\boxed{F'_i = 1 + \frac{\Delta t}{2} \left[ \frac{q_I^{j+1}}{A_i^{j+1}} + \lambda + \frac{k}{d_i^{j+1}} + \alpha \left( 1 - \frac{\text{GAM}^{j+1}}{2 + \text{GAM}^{j+1} + \Delta t \lambda_H + \Delta t \hat{\lambda}_H} \right) \right.} \\ \left. + \rho \hat{\lambda} K_d \left( 1 - \frac{\Delta t \hat{\lambda}}{2 + \Delta t \hat{\lambda}} \right) + \frac{(AD)_{i,i+1}^{j+1} + (AD)_{i-1,i}^{j+1}}{A_i^{j+1} \Delta x^2} \right] \quad (24)$$

$$R''_i = C_i^j + \frac{\Delta t}{2} \left[ \frac{q_I^{j+1}}{A_i^{j+1}} C_I^{j+1} \right. \\ \left. + \alpha \frac{\left(2 - \text{GAM}^j - \Delta t \lambda_H - \Delta t \hat{\lambda}_H\right) C_H^j + \text{GAM}^j C^j + 2\Delta t \hat{\lambda}_H \hat{C}_H + 2\Delta t \gamma}{2 + \text{GAM}^{j+1} + \Delta t \lambda_H + \Delta t \hat{\lambda}_H} \right. \\ \left. + \rho \hat{\lambda} \frac{(2 - \Delta t \hat{\lambda}) C_{\text{sed}}^j + \Delta t \hat{\lambda} K_d C^j}{2 + \Delta t \hat{\lambda}} + G[C, C_H, C_{\text{sed}}]^j \right] \quad (25)$$

## 1.4 Numerical solution - Steady-state

### Finite differences

Using the finite differences approximation shown above (Figure 1), Equation 4 becomes:

$$\begin{aligned}
0 = & - \left( \frac{Q}{A} \right)_i \left( \frac{C_{i+1} - C_{i-1}}{2\Delta x} \right) + \frac{1}{A_i} \left( \frac{(AD)_{i,i+1}(C_{i+1} - C_i) - (AD)_{i-1,i}(C_i - C_{i-1})}{\Delta x^2} \right) \\
& + \frac{q_I}{A_i} (C_I - C_i) - \lambda C_i - \frac{k}{d_i} C_i + \alpha (C_H - C_i) + \rho \hat{\lambda} (C_{\text{sed}} - K_d C_i)
\end{aligned} \tag{26}$$

Substituting Equation 6 and Equation 8 into Equation 26 leads to:

$$\begin{aligned}
0 = & - \left( \frac{Q}{A} \right)_i \left( \frac{C_{i+1} - C_{i-1}}{2\Delta x} \right) + \frac{1}{A_i} \left( \frac{(AD)_{i,i+1}(C_{i+1} - C_i) - (AD)_{i-1,i}(C_i - C_{i-1})}{\Delta x^2} \right) \\
& + \frac{q_I}{A_i} (C_I - C_i) - \lambda C_i - \frac{k}{d_i} C_i + \alpha \left( \frac{\alpha A_i C_i + \gamma A_H + \hat{\lambda}_H \hat{C}_H A_H}{\alpha A_i + \lambda_H A_H + \hat{\lambda}_H A_H} - C_i \right) \\
& + \rho \hat{\lambda} (K_d C_i - K_d C_i) \\
0 = & - \left( \frac{Q}{A} \right)_i \left( \frac{C_{i+1} - C_{i-1}}{2\Delta x} \right) + \frac{1}{A_i} \left( \frac{(AD)_{i,i+1}(C_{i+1} - C_i) - (AD)_{i-1,i}(C_i - C_{i-1})}{\Delta x^2} \right) \\
& + \frac{q_I}{A_i} (C_I - C_i) - \lambda C_i - \frac{k}{d_i} C_i \\
& + \frac{\alpha^2 A_i C_i + \alpha \gamma A_H + \alpha \hat{\lambda}_H \hat{C}_H A_H - \alpha^2 A_i C_i - \alpha \lambda_H A_H C_i - \alpha \hat{\lambda}_H A_H C_i}{\alpha A_i + \lambda_H A_H + \hat{\lambda}_H A_H} \\
0 = & - \left( \frac{Q}{A} \right)_i \left( \frac{C_{i+1} - C_{i-1}}{2\Delta x} \right) + \frac{1}{A_i} \left( \frac{(AD)_{i,i+1}(C_{i+1} - C_i) - (AD)_{i-1,i}(C_i - C_{i-1})}{\Delta x^2} \right) \\
& + \frac{q_I}{A_i} (C_I - C_i) - \lambda C_i - \frac{k}{d_i} C_i + \frac{\alpha A_H (\gamma + \hat{\lambda}_H \hat{C}_H - \lambda_H C_i - \hat{\lambda}_H C_i)}{\alpha A_i + \lambda_H A_H + \hat{\lambda}_H A_H}
\end{aligned} \tag{27}$$

Rearrangement of Equation 27 yields:

$$\boxed{E_i C_{i-1}^{j+1} + F_i C_i^{j+1} + G_i C_{i+1}^{j+1} = R_i} \tag{28}$$

where:

$$\begin{aligned}
E_i C_{i-1} = & \left( \frac{Q}{A} \right)_i \left( \frac{-C_{i-1}}{2\Delta x} \right) - \frac{1}{A_i} \left( \frac{-(AD)_{i-1,i}(-C_{i-1})}{\Delta x^2} \right) \\
\boxed{E_i = & - \frac{1}{A_i \Delta x} \left( \frac{Q_i}{2} + \frac{(AD)_{i-1,i}}{\Delta x} \right)}
\end{aligned} \tag{29}$$

$$\begin{aligned}
F_i C_i = & - \frac{1}{A_i} \left( \frac{(AD)_{i,i+1}(-C_i) - (AD)_{i-1,i}C_i}{\Delta x^2} \right) + \frac{q_I}{A_i} + \lambda C_i + \frac{k}{d_i} C_i \\
& - \frac{\alpha A_H - \lambda_H C_i - \hat{\lambda}_H C_i}{\alpha A_i + \lambda_H A_H + \hat{\lambda}_H A_H} \\
\boxed{F_i = & \frac{(AD)_{i,i+1} + (AD)_{i-1,i}}{A_i \Delta x^2} + \frac{q_I}{A_i} + \lambda + \frac{k}{d_i} + \alpha A_H \frac{\lambda_H + \hat{\lambda}_H}{\alpha A_i + \lambda_H A_H + \hat{\lambda}_H A_H}}
\end{aligned} \tag{30}$$

$$G_i C_{i+1} = \left( \frac{Q}{A} \right)_i \frac{C_{i+1}}{2\Delta x} - \frac{1}{A_i} \left( \frac{(AD)_{i,i+1} C_{i+1}}{\Delta x^2} \right)$$

$$\boxed{G_i = \frac{1}{A_i \Delta x} \left( \frac{Q_i}{2} - \frac{(AD)_{i,i+1}}{\Delta x} \right)} \quad (31)$$

$$\boxed{R_i = \frac{q_I}{A_i} C_I + \frac{\alpha A_H (\gamma + \hat{\lambda}_H \hat{C}_H)}{\alpha A_i + \lambda_H A_H + \hat{\lambda}_H A_H}} \quad (32)$$

### 1.5 Solving the numerical equations

Equation 14 and Equation 28 can be solved as:

$$\begin{bmatrix} F_1^{(j)} & G_1 & & & \\ E_2 & F_2^{(j)} & G_2 & & \\ & & \dots & & \\ & & E_{N-1} & F_{N-1}^{(j)} & G_{N-1} \\ & & & E_N & F_N^{(j)} \end{bmatrix} \begin{bmatrix} C_1^{j+1} \\ C_2^{j+1} \\ \dots \\ C_{N-1}^{j+1} \\ C_N^{j+1} \end{bmatrix} = \begin{bmatrix} R_1^{(j)} \\ R_2^{(j)} \\ \dots \\ R_{N-1}^{(j)} \\ R_N^{(j)} \end{bmatrix} \quad (33)$$

where  $N$  is the number of segments.

### Bibliography

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