

McMaster University Winter 2021  
**CIVENG 4V04: Term Project**  
Activated Sludge Model Development (Part A)

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# Mass Balances on Soluble Components

## Mass Balance on Soluble Substrates

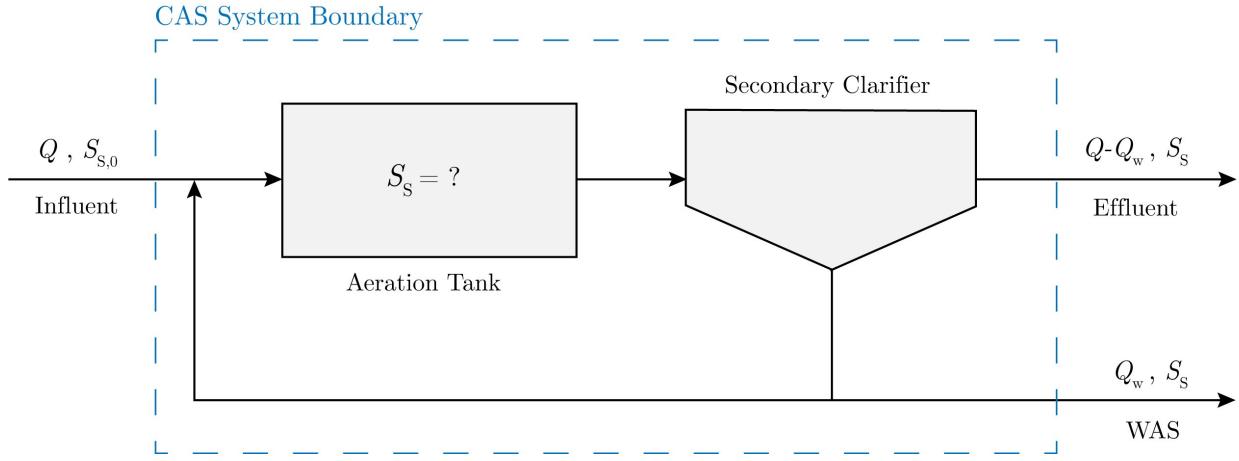


Figure 1: Schematic diagram of the mass balance set-up for  $S_S$  assuming an Activated Sludge System.

Given the CAS system depicted in Figure 1 above:

- (i) Let  $S_S$  denote the effluent soluble substrate concentration (in mg-COD/L);
- (ii) Let  $S_{S,0}$  denote influent soluble substrate concentration (in mg-COD/L);
- (iii) Let  $Q$  denote the flowrate of the influent (in  $\text{m}^3/\text{d}$ );
- (iv) Let  $Q_w$  denote the waste sludge flowrate (in  $\text{m}^3/\text{d}$ ).

To begin performing a mass balance on  $S_S$ , we make note of our first assumption (which has already been depicted in Figure 1). That is, in the secondary clarifier, *no separation* of soluble components occurs (i.e., WAS and effluent  $S_S$  concentrations are the same). Now, by applying the Law of Conservation of Mass on the defined system boundary to determine  $S_S$ , we obtain

$$\begin{aligned}
 [\text{Change}] &= [\text{Inlet}] - [\text{Outlet}] + [\text{Reaction Expression(s)}] \\
 V \cdot \frac{dS_S}{dt} &= QS_{S,0} - [(Q - Q_w)S_S + Q_wS_S] + [\text{Reaction Expression(s)}] \\
 V \cdot \frac{dS_S}{dt} &= QS_{S,0} - QS_S + Q_wS_S - Q_wS_S + [\text{Reaction Expression(s)}] \\
 V \cdot \frac{dS_S}{dt} &= Q(S_{S,0} - S_S) + [\text{Reaction Expression(s)}].
 \end{aligned} \tag{1}$$

Applying the steady state assumption to the equation above implies that  $\frac{dS_S}{dt} = 0$ . So equation (1) simplifies

to the following

$$0 = Q(S_{S,0} - S_S) + [\text{Reaction Expression}(s)]. \quad (2)$$

To determine the reaction terms in equation (2), we first refer to Figure 2 below.

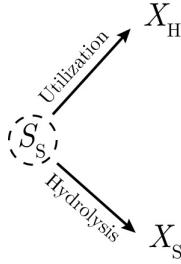


Figure 2: Reaction diagram in the perspective of  $S_S$  developed from the reaction chart provided for the term project on Avenue to Learn.

Based on the kinetic expressions associated with each of the individual reactions shown above, we have

$$\begin{aligned} [\text{Reaction}] &= V \cdot \frac{dS_S}{dt} \Big|_{\text{Utilization}} + V \cdot \frac{dS_S}{dt} \Big|_{\text{Hydrolysis}} \\ &= V \left( \frac{dS_S}{dt} \Big|_{\text{Utilization}} + \frac{dS_S}{dt} \Big|_{\text{Hydrolysis}} \right) \\ [\text{Reaction}] &= V \left\{ -\frac{1}{Y_H} \left[ \mu_{m,H} \left( \frac{S_S}{K_{SS} + S_S} \right) \left( \frac{S_O}{K_O^H + S_O} \right) X_H \right. \right. \\ &\quad \left. \left. + \mu_{m,H} \left( \frac{S_S}{K_{SS} + S_S} \right) \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{K_O^H}{K_O^H + S_O} \right) 0.8X_H \right] - (-k_h X_S X_H) \right\} \\ [\text{Reaction}] &= V \left\{ -\frac{1}{Y_H} \mu_{m,H} X_H \left( \frac{S_S}{K_{SS} + S_S} \right) \left( \frac{1}{K_O^H + S_O} \right) \left[ S_O + 0.8K_O^H \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \right] + k_h X_S X_H \right\} \end{aligned} \quad (3)$$

Substituting equation (3) into equation (2) yields the following

$$0 = Q(S_{S,0} - S_S) + V \left\{ -\frac{1}{Y_H} \mu_{m,H} X_H \left( \frac{S_S}{K_{SS} + S_S} \right) \left( \frac{1}{K_O^H + S_O} \right) \left[ S_O + 0.8K_O^H \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \right] + k_h X_S X_H \right\}$$

Dividing both sides of the equation above by  $V$ , we obtain

$$0 = \frac{Q}{V}(S_{S,0} - S_S) - \frac{1}{Y_H}\mu_{m,H}X_H\left(\frac{S_S}{K_{SS} + S_S}\right)\left(\frac{1}{K_O^H + S_O}\right)\left[S_O + 0.8K_O^H\left(\frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}\right)\right] + k_h X_S X_H. \quad (4)$$

By definition,

$$\frac{1}{\theta} = \frac{Q}{V}. \quad (5)$$

Substituting equation (5) into equation (4) as follows

$$\begin{aligned} 0 &= \frac{1}{\theta}(S_{S,0} - S_S) - \frac{1}{Y_H}\mu_{m,H}X_H\left(\frac{S_S}{K_{SS} + S_S}\right)\left(\frac{1}{K_O^H + S_O}\right)\left[S_O + 0.8K_O^H\left(\frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}\right)\right] + k_h X_S X_H \\ 0 &= \frac{1}{\theta}S_{S,0} - \frac{1}{\theta}S_S - \frac{1}{Y_H}\mu_{m,H}X_H\left(\frac{S_S}{K_{SS} + S_S}\right)\left(\frac{1}{K_O^H + S_O}\right)\left[S_O + 0.8K_O^H\left(\frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}\right)\right] + k_h X_S X_H \\ 0 &= \frac{1}{\theta}S_{S,0} - S_S \left\{ \frac{1}{\theta} + \frac{1}{Y_H}\mu_{m,H}X_H\left(\frac{1}{K_{SS} + S_S}\right)\left(\frac{1}{K_O^H + S_O}\right)\left[S_O + 0.8K_O^H\left(\frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}\right)\right] \right\} + k_h X_S X_H, \end{aligned}$$

and re-arranging to solve for  $S_S$  results in

$$\begin{aligned} \frac{1}{\theta}S_{S,0} + k_h X_S X_H &= S_S \left\{ \frac{1}{\theta} + \frac{1}{Y_H}\mu_{m,H}X_H\left(\frac{1}{K_{SS} + S_S}\right)\left(\frac{1}{K_O^H + S_O}\right)\left[S_O + 0.8K_O^H\left(\frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}\right)\right] \right\} \\ \theta S_S &= \frac{\theta \left( \frac{1}{\theta}S_{S,0} + k_h X_S X_H \right)}{\frac{1}{\theta} + \frac{1}{Y_H}\mu_{m,H}X_H\left(\frac{1}{K_{SS} + S_S}\right)\left(\frac{1}{K_O^H + S_O}\right)\left[S_O + 0.8K_O^H\left(\frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}\right)\right]}. \end{aligned}$$

Therefore,

$$S_S = \boxed{\frac{S_{S,0} + \theta k_h X_S X_H}{1 + \theta \left\{ \frac{1}{Y_H}\mu_{m,H}X_H\left(\frac{1}{K_{SS} + S_S}\right)\left(\frac{1}{K_O^H + S_O}\right)\left[S_O + 0.8K_O^H\left(\frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}\right)\right] \right\}}}$$

# Mass Balances on Particulate Components

## Mass Balance on Particulate Substrates

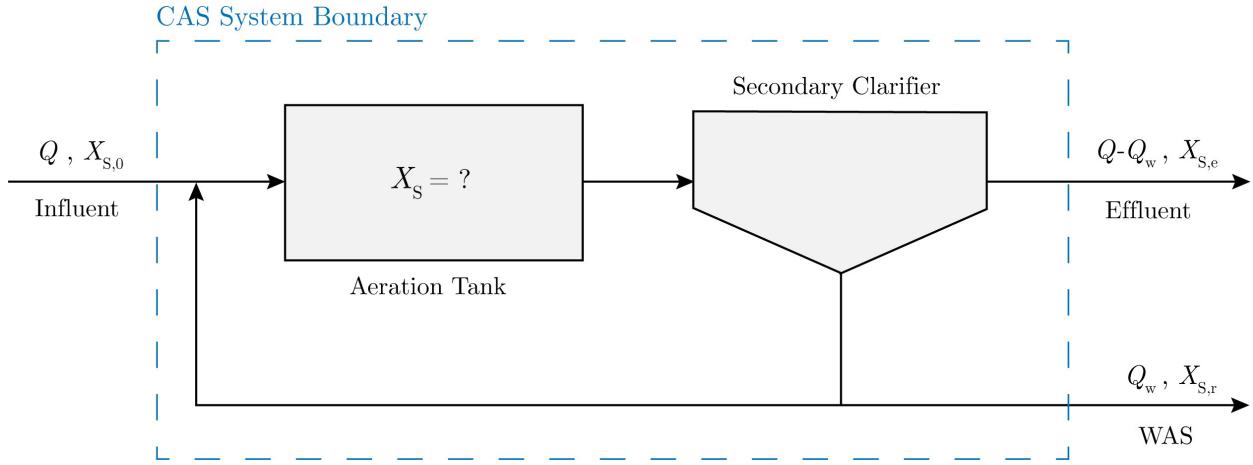


Figure 3: Schematic diagram of the mass balance set-up for  $X_S$  assuming an Activated Sludge System.

Given the CAS system depicted in Figure 3 above:

- (i) Let  $X_{S,e}$  denote the effluent particulate substrate concentration (in mg-COD/L);
- (ii) Let  $X_{S,r}$  denote the WAS particulate substrate concentration (in mg-COD/L);
- (iii) Let  $X_{S,0}$  denote influent particulate substrate concentration (in mg-COD/L);
- (iv) Let  $Q$  denote the flowrate of the influent ( $\text{m}^3/\text{d}$ );
- (v) Let  $Q_w$  denote the waste sludge flowrate ( $\text{m}^3/\text{d}$ ).

To begin performing a mass balance on the particulate substrate concentration,  $X_S$ , we apply the Law of Conservation of Mass on the system boundary. Doing so yields

$$\begin{aligned}
 [\text{Change}] &= [\text{Inlet}] - [\text{Outlet}] + [\text{Reaction}] \\
 V \cdot \frac{dX_S}{dt} &= QX_{S,0} - [(Q - Q_w)X_{S,e} + Q_wX_{S,r}] + [\text{Reaction}] \\
 V \cdot \frac{dX_S}{dt} &= QX_{S,0} - QX_{S,e} + Q_wX_{S,e} - Q_wX_{S,r} + [\text{Reaction}].
 \end{aligned} \tag{6}$$

Applying the steady state assumption to the equation above implies that  $\frac{dX_S}{dt} = 0$ . So equation (6) simplifies to the following

$$0 = QX_{S,0} - QX_{S,e} + Q_wX_{S,e} - Q_wX_{S,r} + [\text{Reaction}]. \tag{7}$$

Additionally, assuming that

$$\left. \frac{X_S}{X_{\text{Total}}} \right|_{\text{Bioreactor}} = \frac{X_{S,e}}{X_{\text{Total},e}} = \frac{X_{S,r}}{X_{\text{Total},r}},$$

equation (7) may be simplified as follows

$$\begin{aligned} 0 &= QX_{S,0} - QX_S \frac{X_{\text{Total},e}}{X_{\text{Total}}} + Q_w X_S \frac{X_{\text{Total},e}}{X_{\text{Total}}} - Q_w X_S \frac{X_{\text{Total},r}}{X_{\text{Total}}} + [\text{Reaction}] \\ 0 &= QX_{S,0} - X_S \left[ \frac{(Q - Q_w)X_{\text{Total},e} + Q_w X_{\text{Total},r}}{X_{\text{Total}}} \right] + [\text{Reaction}]. \end{aligned} \quad (8)$$

To determine the reaction term in (8), we first refer to Figure 4 below.

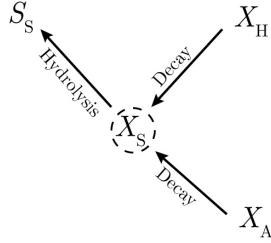


Figure 4: Reaction diagram in the perspective of  $X_S$  developed from the reaction chart provided for the term project on Avenue to Learn.

Based on the kinetic expressions associated with each of the individual reactions shown above, we have

$$\begin{aligned} [\text{Reaction}] &= V \cdot \left. \frac{dX_S}{dt} \right|_{\text{Hydrolysis}} + V \cdot \left. \frac{dX_S}{dt} \right|_{\text{Decay}} \\ &= V \left( \left. \frac{dX_S}{dt} \right|_{\text{Hydrolysis}} + \left. \frac{dX_S}{dt} \right|_{\text{Decay}} \right) \\ &= V \left[ -k_h X_S X_H + (1 - f_d) \left( -\left. \frac{dX_H}{dt} \right|_{\text{Decay}} - \left. \frac{dX_A}{dt} \right|_{\text{Decay}} - \left. \frac{dX_{\text{NOB}}}{dt} \right|_{\text{Decay}} \right) \right] \\ &= V \left( \left. \frac{dX_S}{dt} \right|_{\text{Hydrolysis}} + \left. \frac{dX_S}{dt} \right|_{\text{Decay}} \right) \\ &= V \left[ -k_h X_S X_H + (1 - f_d)(b_H X_H + b_A X_A) \right]. \end{aligned} \quad (9)$$

Substituting the result of equation (9) into equation (8) results in

$$0 = QX_{S,0} - X_S \left[ \frac{(Q - Q_w)X_{\text{Total,e}} + Q_wX_{\text{Total,r}}}{X_{\text{Total}}} \right] + V \left[ -k_h X_S X_H + (1 - f_d)(b_H X_H + b_A X_A) \right]. \quad (10)$$

Dividing both sides of equation (10) by  $V$ , we obtain

$$0 = \frac{Q}{V}X_{S,0} - X_S \left[ \frac{(Q - Q_w)X_{\text{Total,e}} + Q_wX_{\text{Total,r}}}{V \cdot X_{\text{Total}}} \right] + \left[ -k_h X_S X_H + (1 - f_d)(b_H X_H + b_A X_A) \right]. \quad (11)$$

By definition,

$$\frac{1}{\theta} = \frac{Q}{V} \quad \text{and} \quad \frac{1}{\theta_c} = \frac{(Q - Q_w)X_{\text{Total,e}} + Q_wX_{\text{Total,r}}}{V \cdot X_{\text{Total}}}. \quad (12)$$

Substituting both equations defined in (12) into equation (11) and re-arranging the resultant equation so as to solve for  $X_S$  yields

$$\begin{aligned} 0 &= \frac{1}{\theta}X_{S,0} - \frac{1}{\theta_c}X_S - [k_h X_S X_H] + [(1 - f_d)(b_H X_H + b_A X_A)] \\ \frac{1}{\theta_c}X_S + [k_h X_S X_H] &= \frac{1}{\theta}X_{S,0} + [(1 - f_d)(b_H X_H + b_A X_A)] \\ X_S \left( \frac{1}{\theta_c} + [k_h X_H] \right) &= \frac{1}{\theta}X_{S,0} + [(1 - f_d)(b_H X_H + b_A X_A)]. \end{aligned}$$

Therefore, we obtain that

$$X_S = \frac{\frac{1}{\theta}X_{S,0} + [(1 - f_d)(b_H X_H + b_A X_A)]}{\left( \frac{1}{\theta_c} + [k_h X_H] \right)}$$

## Mass Balance on Inert Solids

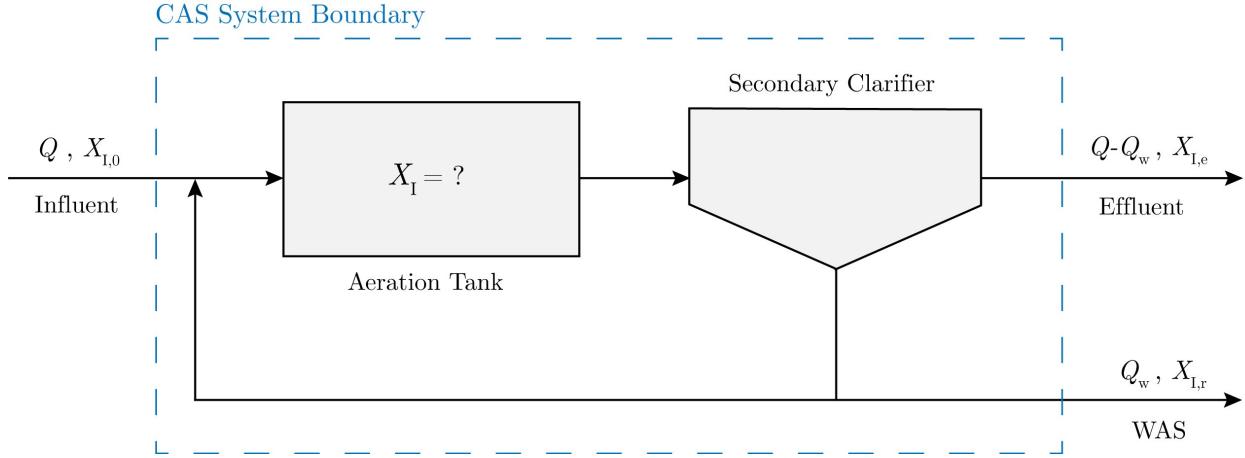


Figure 5: Schematic diagram of the mass balance set-up for  $X_I$  assuming an Activated Sludge System.

Given the CAS system depicted in Figure 5 above:

- (i) Let  $X_{I,e}$  denote the effluent inert solids concentration (in mg-COD/L);
- (ii) Let  $X_{I,r}$  denote the WAS inert solids concentration (in mg-COD/L);
- (iii) Let  $X_{I,0}$  denote influent inert solids concentration (in mg-COD/L);
- (iv) Let  $Q$  denote the flowrate of the influent (in  $\text{m}^3/\text{d}$ );
- (v) Let  $Q_w$  denote the waste sludge flowrate (in  $\text{m}^3/\text{d}$ ).

To begin performing a mass balance on the particulate substrate concentration,  $X_I$ , we apply the Law of Conservation of Mass on the system boundary. Doing so yields

$$\begin{aligned} [\text{Change}] &= [\text{Inlet}] - [\text{Outlet}] + [\text{Reaction}] \\ V \cdot \frac{dX_I}{dt} &= QX_{I,0} - [(Q - Q_w)X_{I,e} + Q_wX_{I,r}] + [\text{Reaction}] \\ V \cdot \frac{dX_I}{dt} &= QX_{I,0} - QX_{I,e} + Q_wX_{I,e} - Q_wX_{I,r} + [\text{Reaction}]. \end{aligned} \quad (13)$$

Applying the steady state assumption to the equation above implies that  $\frac{dX_I}{dt} = 0$ . So equation (13) simplifies to the following

$$0 = QX_{I,0} - QX_{I,e} + Q_wX_{I,e} - Q_wX_{I,r} + [\text{Reaction}]. \quad (14)$$

Additionally, assuming that

$$\left. \frac{X_I}{X_{\text{Total}}} \right|_{\text{Bioreactor}} = \frac{X_{I,e}}{X_{\text{Total},e}} = \frac{X_{I,r}}{X_{\text{Total},r}},$$

equation (14) may be simplified as follows

$$\begin{aligned} 0 &= QX_{I,0} - QX_I \frac{X_{\text{Total},e}}{X_{\text{Total}}} + Q_w X_I \frac{X_{\text{Total},e}}{X_{\text{Total}}} - Q_w X_I \frac{X_{\text{Total},r}}{X_{\text{Total}}} + [\text{Reaction}] \\ 0 &= QX_{I,0} - X_I \left[ \frac{(Q - Q_w)X_{\text{Total},e} + Q_w X_{\text{Total},r}}{X_{\text{Total}}} \right] + [\text{Reaction}]. \end{aligned} \quad (15)$$

To determine the reaction term in (15), we first refer to the reaction chart provided on Avenue to Learn. Based on the kinetic expressions associated with each of the reactions, we have that

$$\begin{aligned} [\text{Reaction}] &= V \cdot \left. \frac{dX_I}{dt} \right|_{\text{Decay}} \\ &= V \cdot f_d \left( - \left. \frac{dX_H}{dt} \right|_{\text{Decay}} - \left. \frac{dX_A}{dt} \right|_{\text{Decay}} \right) \\ &= V \cdot f_d(b_H X_H + b_A X_A). \end{aligned} \quad (16)$$

Substituting the result of equation (16) into equation (15) results in

$$0 = QX_{I,0} - X_I \left[ \frac{(Q - Q_w)X_{\text{Total},e} + Q_w X_{\text{Total},r}}{X_{\text{Total}}} \right] + V \cdot f_d(b_H X_H + b_A X_A). \quad (17)$$

Dividing both sides of equation (17) by  $V$ , we obtain

$$0 = \frac{Q}{V} X_{I,0} - X_I \left[ \frac{(Q - Q_w)X_{\text{Total},e} + Q_w X_{\text{Total},r}}{V \cdot X_{\text{Total}}} \right] + f_d(b_H X_H + b_A X_A). \quad (18)$$

By definition,

$$\frac{1}{\theta} = \frac{Q}{V} \quad \text{and} \quad \frac{1}{\theta_c} = \frac{(Q - Q_w)X_{\text{Total},e} + Q_w X_{\text{Total},r}}{V \cdot X_{\text{Total}}}. \quad (19)$$

Substituting both equations defined in (19) into equation (18) and re-arranging the resultant equation so as to solve for  $X_I$  yields

$$\begin{aligned} 0 &= \frac{1}{\theta} X_{I,0} - \frac{1}{\theta_c} X_I + f_d(b_H X_H + b_A X_A) \\ \frac{1}{\theta_c} X_I &= \frac{1}{\theta} X_{I,0} + f_d(b_H X_H + b_A X_A). \end{aligned}$$

Therefore, we have that

$$X_I = \boxed{\frac{\frac{1}{\theta} X_{I,0} + f_d(b_H X_H + b_A X_A)}{\frac{1}{\theta_c}}}$$

## Mass Balance on Particulate Organic Nitrogen

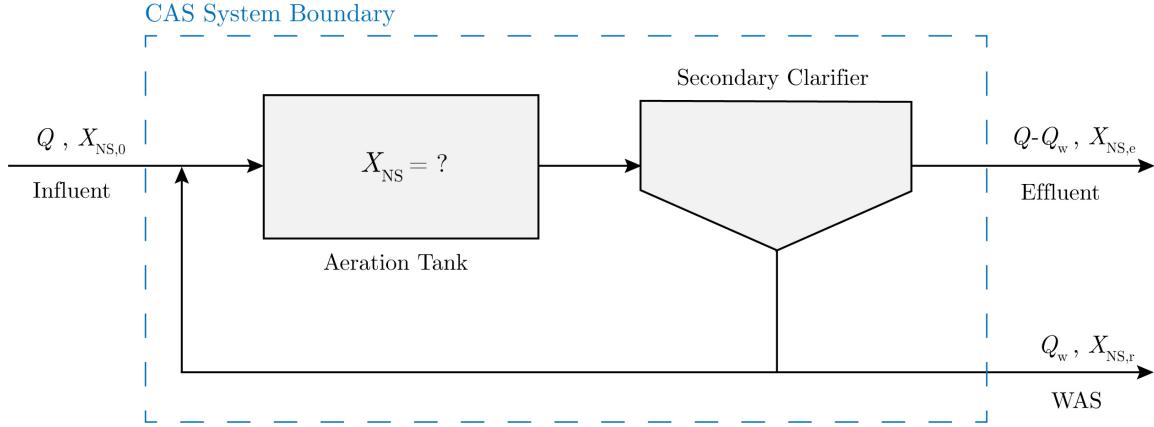


Figure 6: Schematic diagram of the mass balance set-up for  $X_{NS}$  assuming an Activated Sludge System.

Given the CAS system depicted in Figure 6 above:

- (i) Let  $X_{NS,e}$  denote the effluent particulate organic nitrogen concentration (in mg-N/L);
- (ii) Let  $X_{NS,r}$  denote the WAS particulate organic nitrogen concentration (in mg-N/L);
- (iii) Let  $X_{NS,0}$  denote influent inert particulate organic nitrogen concentration (in mg-N/L);
- (iv) Let  $Q$  denote the flowrate of the influent (in m<sup>3</sup>/d);
- (v) Let  $Q_w$  denote the waste sludge flowrate (in m<sup>3</sup>/d).

To begin performing a mass balance on  $X_{NS}$ , we apply the Law of Conservation of Mass on the system boundary. Doing so yields

$$\begin{aligned}
 [\text{Change}] &= [\text{Inlet}] - [\text{Outlet}] + [\text{Reaction}] \\
 V \cdot \frac{dX_{NS}}{dt} &= QX_{NS,0} - [(Q - Q_w)X_{NS,e} + Q_wX_{NS,r}] + [\text{Reaction}] \quad (20) \\
 V \cdot \frac{dX_{NS}}{dt} &= QX_{NS,0} - QX_{NS,e} + Q_wX_{NS,e} - Q_wX_{NS,r} + [\text{Reaction}].
 \end{aligned}$$

Applying the steady state assumption to the equation above implies that  $\frac{dX_{NS}}{dt} = 0$ . So equation (20) simplifies to the following

$$0 = QX_{NS,0} - QX_{NS,e} + Q_wX_{NS,e} - Q_wX_{NS,r} + [\text{Reaction}]. \quad (21)$$

Additionally, assuming that

$$\left. \frac{X_{\text{NS}}}{X_{\text{Total}}} \right|_{\text{Bioreactor}} = \frac{X_{\text{NS,e}}}{X_{\text{Total,e}}} = \frac{X_{\text{NS,r}}}{X_{\text{Total,r}}},$$

equation (21) may be simplified as follows

$$\begin{aligned} 0 &= QX_{\text{NS},0} - QX_{\text{NS}} \frac{X_{\text{Total,e}}}{X_{\text{Total}}} + Q_w X_{\text{NS}} \frac{X_{\text{Total,e}}}{X_{\text{Total}}} - Q_w X_{\text{NS}} \frac{X_{\text{Total,r}}}{X_{\text{Total}}} + [\text{Reaction}] \\ 0 &= QX_{\text{NS},0} - X_{\text{NS}} \left[ \frac{(Q - Q_w)X_{\text{Total,e}} + Q_w X_{\text{Total,r}}}{X_{\text{Total}}} \right] + [\text{Reaction}]. \end{aligned} \quad (22)$$

To determine the reaction term in (22), we first refer to the reaction chart provided on Avenue to Learn. Based on the kinetic expressions associated with each of the reactions, we have that

$$\begin{aligned} [\text{Reaction}] &= V \cdot \left[ \frac{X_{\text{NS}}}{X_S} (-k_h X_S X_H) + i_{N/\text{decay}} (b_H X_H + b_A X_A) \right] \\ &= V \cdot [X_{\text{NS}} (-k_h X_H) + i_{N/\text{decay}} (b_H X_H + b_A X_A)]. \end{aligned} \quad (23)$$

Substituting the result of equation (23) into equation (22) results in

$$0 = QX_{\text{NS},0} - X_{\text{NS}} \left[ \frac{(Q - Q_w)X_{\text{Total,e}} + Q_w X_{\text{Total,r}}}{X_{\text{Total}}} \right] + V \cdot [X_{\text{NS}} (-k_h X_H) + i_{N/\text{decay}} (b_H X_H + b_A X_A)]. \quad (24)$$

Dividing both sides of equation (24) by  $V$ , we obtain

$$0 = \frac{Q}{V} X_{\text{NS},0} - X_{\text{NS}} \left[ \frac{(Q - Q_w)X_{\text{Total,e}} + Q_w X_{\text{Total,r}}}{V \cdot X_{\text{Total}}} \right] + [X_{\text{NS}} (-k_h X_H) + i_{N/\text{decay}} (b_H X_H + b_A X_A)]. \quad (25)$$

By definition,

$$\frac{1}{\theta} = \frac{Q}{V} \quad \text{and} \quad \frac{1}{\theta_c} = \frac{(Q - Q_w)X_{\text{Total,e}} + Q_w X_{\text{Total,r}}}{V \cdot X_{\text{Total}}}. \quad (26)$$

Substituting both equations defined in (26) into equation (25) and re-arranging the resultant equation so as

to solve for  $X_{\text{NS}}$  yields

$$0 = \frac{1}{\theta} X_{\text{NS},0} - \frac{1}{\theta_c} X_{\text{NS}} + [X_{\text{NS}}(-k_h X_{\text{H}}) + i_{N/\text{decay}}(b_{\text{H}} X_{\text{H}} + b_{\text{A}} X_{\text{A}})].$$

Therefore, we have that

$$X_{\text{NS}} = \boxed{\frac{\frac{1}{\theta} X_{\text{NS},0} + i_{N/\text{decay}}(b_{\text{H}} X_{\text{H}} + b_{\text{A}} X_{\text{A}})}{\frac{1}{\theta_c} + k_h X_{\text{H}}}}$$

## MASS BALANCE ON AUTOTROPHIC MICROORGANISMS ( $X_A$ )

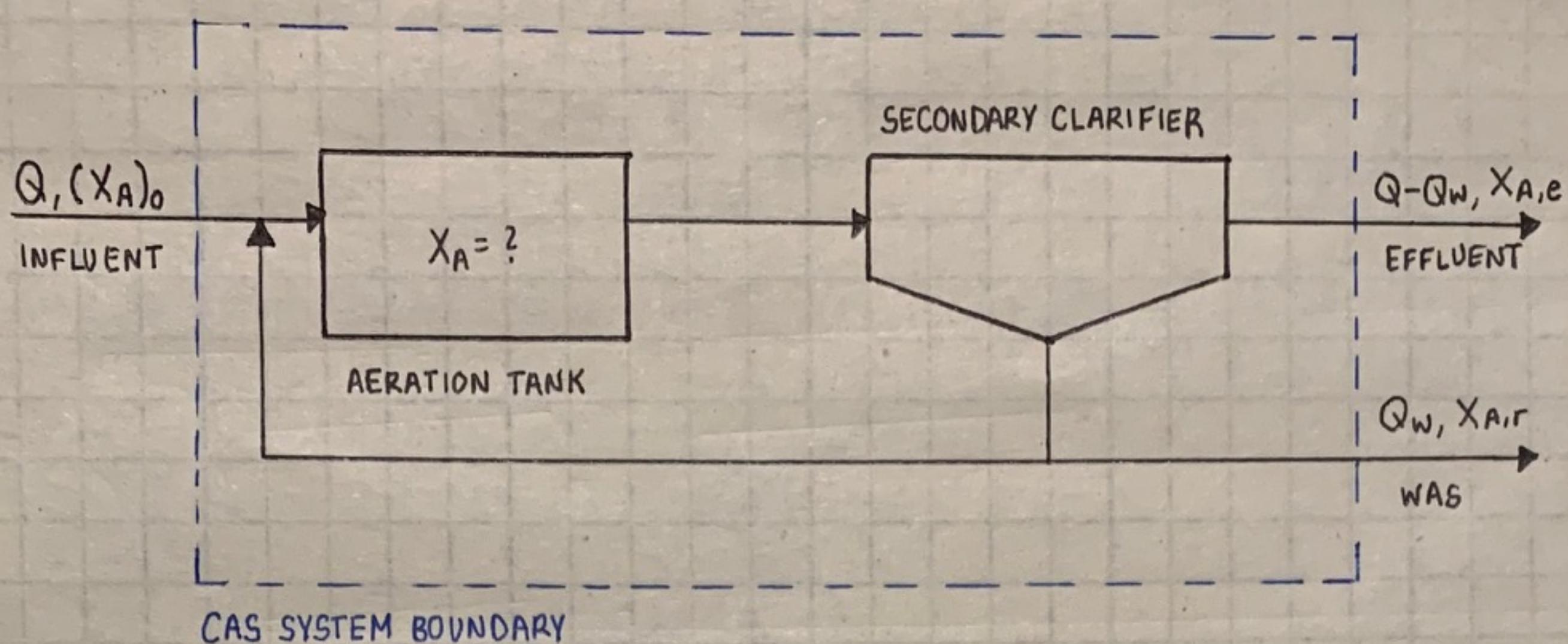


FIGURE 1: Schematic diagram of the mass balance set-up for  $X_A$  assuming an Activated Sludge System.

Given the CAS system depicted in FIGURE 1 above :

- (i) Let  $X_{A,e}$  denote the effluent autotrophic microorganism concentration (in mg-COD/L);
- (ii) Let  $X_{A,r}$  denote the WAS autotrophic microorganism concentration (in mg-COD/L);
- (iii) Let  $X_{A,0}$  denote the influent autotrophic microorganism concentration (in mg-COD/L);
- (iv) Let  $Q$  denote the flowrate of the influent (in  $m^3/d$ );
- (v) Let  $Q_w$  denote the waste sludge flowrate (in  $m^3/d$ ).

To begin performing a mass balance on  $X_A$ , we apply the Law of Conservation of Mass on the system boundary. Doing so results in

$$[\text{Change}] = [\text{Inlet}] - [\text{Outlet}] + [\text{Reaction}]$$

$$V \cdot \frac{dX_A}{dt} = Q X_{A,0} - [(Q - Q_w) X_{A,e} + Q_w X_{A,r}] + [\text{Reaction}]$$

$$V \cdot \frac{dX_A}{dt} = Q X_{A,0} - Q X_{A,e} + Q_w X_{A,e} - Q_w X_{A,r} + [\text{Reaction}] \quad (1)$$

Applying the steady state assumption to the above equation implies that  $dX_A/dt = 0$ . So equation (1) will simplify as follows

$$0 = Q X_{A,0} - Q X_{A,e} + Q_w X_{A,e} + Q_w X_{A,r} + [\text{Reaction}] \quad (2)$$

Also, assuming that the separation of  $X_A$  in the bioreactor is equal to that of  $X_A$  in the effluent and to  $X_A$  in WAS :

$$\left. \frac{X_A}{X_{\text{TOTAL}}} \right|_{\text{BIOREACTOR}} = \frac{X_{A,e}}{X_{\text{TOTAL},e}} = \frac{X_{A,r}}{X_{\text{TOTAL},r}},$$

equation (2) may be further simplified as follows (see next page).

$$0 = QX_{A,0} - QX_A \left( \frac{X_{\text{TOTAL},e}}{X_{\text{TOTAL}}} \right) + Q_w X_A \left( \frac{X_{\text{TOTAL},e}}{X_{\text{TOTAL}}} \right) - Q_w X_A \left( \frac{X_{\text{TOTAL},r}}{X_{\text{TOTAL}}} \right) + [\text{Reaction}]$$

$$0 = QX_{A,0} - X_A \left[ \frac{(Q-Q_w)X_{\text{TOTAL},e} + Q_w X_{\text{TOTAL},r}}{X_{\text{TOTAL}}} \right] + [\text{Reaction}] \quad (3)$$

To determine the reaction term in equation (3), we refer to FIGURE 2 below.

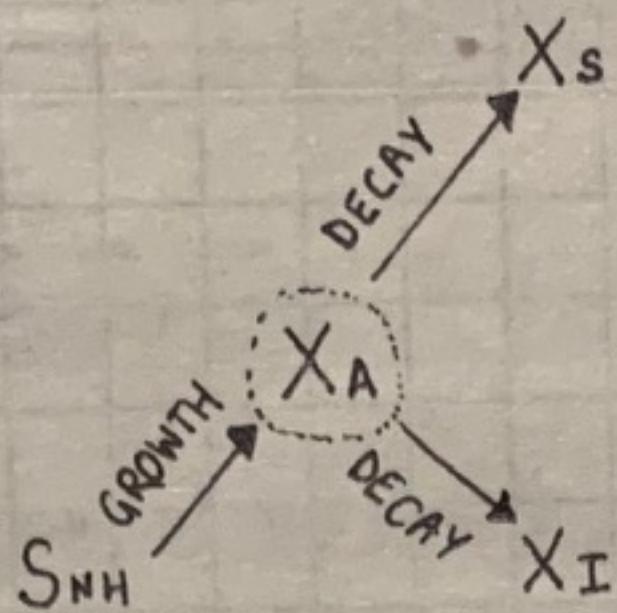


FIGURE 2: Reaction diagram in the perspective of  $X_A$  developed from the reaction chart provided for the term project on Avenue to Learn.

Based on the Kinetic expressions associated with each of the individual reactions shown above, we have

$$\begin{aligned} [\text{Reaction}] &= V \cdot \frac{dX_A}{dt} \Big|_{\text{GROWTH}} + V \cdot \frac{dX_A}{dt} \Big|_{\text{DECAY}} \\ &= V \left( \frac{dX_A}{dt} \Big|_{\text{GROWTH}} + \frac{dX_A}{dt} \Big|_{\text{DECAY}} \right) \\ &= V \left[ \mu_{m,A} \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_0^A + S_0} \right) X_A - b_A X_A \right] \end{aligned} \quad (4)$$

Substituting equation (4) into equation (3) yields

$$0 = QX_{A,0} - X_A \left[ \frac{(Q-Q_w)X_{\text{TOTAL},e} + Q_w X_{\text{TOTAL},r}}{X_{\text{TOTAL}}} \right] + V \left[ \mu_{m,A} \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_0^A + S_0} \right) X_A - b_A X_A \right] \quad (5)$$

Dividing both sides of equation (5) by  $V$ , we obtain

$$\cancel{\frac{1}{V}} X_{A,0} - X_A \left[ \frac{(Q-Q_w)X_{\text{TOTAL},e} + Q_w X_{\text{TOTAL},r}}{V \cdot X_{\text{TOTAL}}} \right] + \mu_{m,A} \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_0^A + S_0} \right) X_A - b_A X_A \rightarrow \frac{1}{\theta_c}$$

$$0 = \frac{1}{\theta} X_{A,0} - \frac{1}{\theta_c} X_A + \mu_{m,A} \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_0^A + S_0} \right) X_A - b_A X_A$$

$$\frac{1}{\theta_c} X_A + b_A X_A = \frac{1}{\theta} X_{A,0} + \mu_{m,A} \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_0^A + S_0} \right) X_A.$$

Therefore, we have

$$X_A = \frac{\frac{1}{\theta} X_{A,0} + \mu_{m,A} \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_0^A + S_0} \right) X_A}{\left( \frac{1}{\theta_c} + b_A \right)}$$

## MASS BALANCE ON NITRATE NITROGEN ( $\text{NO}_3^-$ )

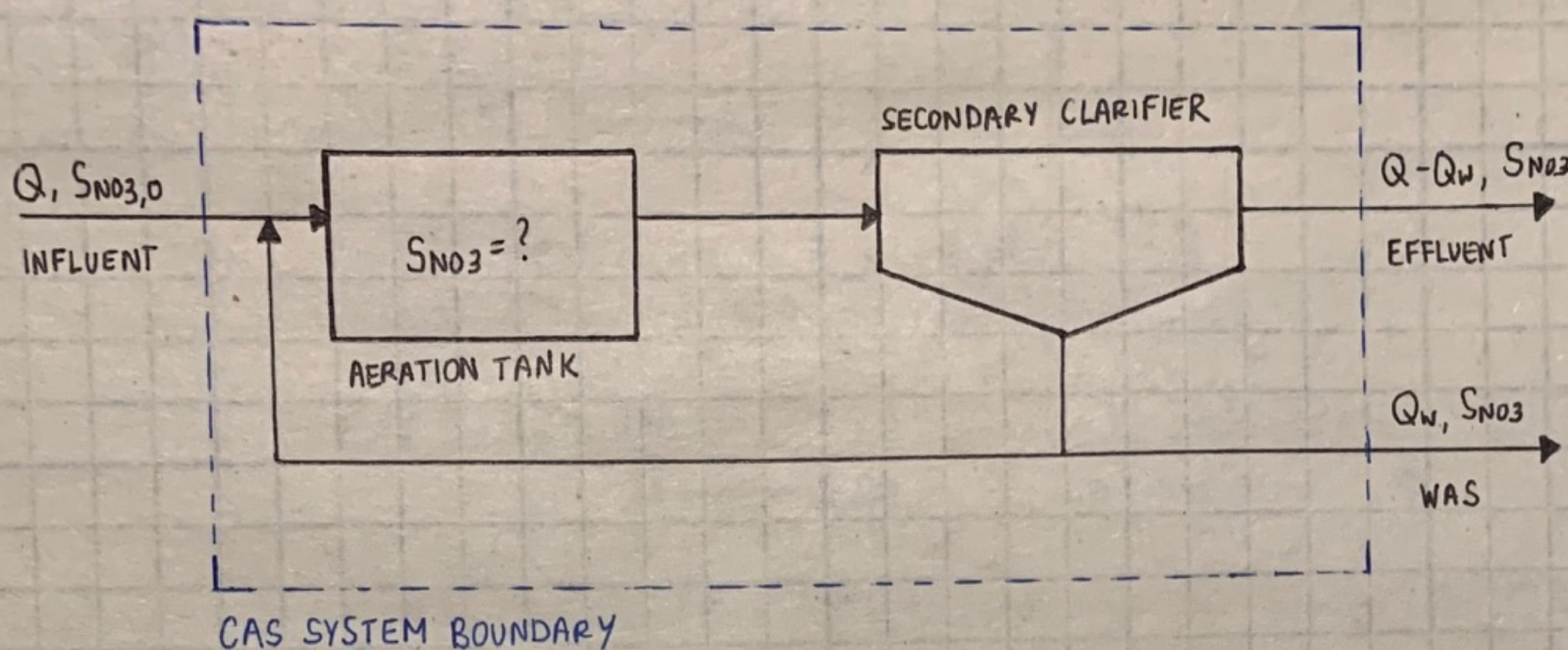


FIGURE 3: Schematic diagram of the mass balance set-up for  $\text{NO}_3^-$  assuming an Activated Sludge System.

Given the CAS system depicted in FIGURE 3 above:

- (i) Let  $S_{\text{NO}_3,0}$  denote the influent nitrate nitrogen concentration (in mg-N/L);
- (ii) Let  $S_{\text{NO}_3}$  denote the effluent nitrate nitrogen concentration (in mg-N/L);
- (iii) Let  $Q$  denote the flowrate of the influent (in  $\text{m}^3/\text{d}$ );
- (iv) Let  $Q_w$  denote the WAS flowrate (in  $\text{m}^3/\text{d}$ ).

To begin performing a mass balance on  $\text{NO}_3^-$ , we make note of our first assumption (which has already been depicted in the schematic above). That is, in the secondary clarifier, no separation of soluble components occurs (i.e., WAS and effluent  $\text{NO}_3^-$  concentrations are equal). Now, by applying Conservation of Mass on the system boundary, we obtain

$$[\text{Change}] = [\text{Inlet}] - [\text{Outlet}] + [\text{Reaction}]$$

$$V \cdot \frac{dS_{\text{NO}_3}}{dt} = Q S_{\text{NO}_3,0} - [(Q - Q_w) S_{\text{NO}_3} + Q_w S_{\text{NO}_3}] + [\text{Reaction}]$$

$$V \cdot \frac{dS_{\text{NO}_3}}{dt} = Q S_{\text{NO}_3,0} - Q S_{\text{NO}_3} + Q_w S_{\text{NO}_3} - Q_w S_{\text{NO}_3} + [\text{Reaction}]$$

$$V \cdot \frac{dS_{\text{NO}_3}}{dt} = Q (S_{\text{NO}_3,0} - S_{\text{NO}_3}) + [\text{Reaction}] \quad (6)$$

Applying steady state assumptions on (6) implies  $dS_{\text{NO}_3}/dt = 0$  and so we obtain

$$0 = Q (S_{\text{NO}_3,0} - S_{\text{NO}_3}) + [\text{Reaction}] \quad (7)$$

To determine the reaction term in equation (7), we first refer to FIGURE 4 below.

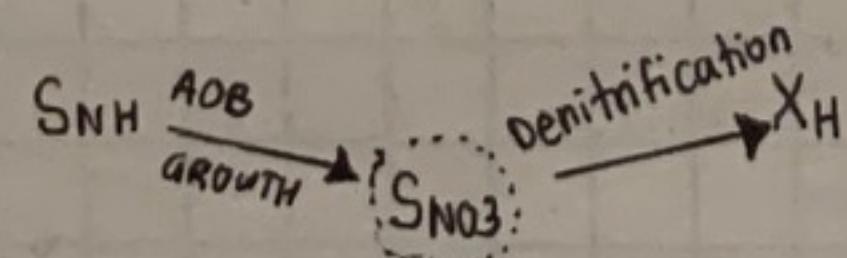


FIGURE 4: Reaction diagram in the perspective of  $\text{NO}_3^-$  developed from the term project reaction chart.

Based on the kinetic expressions associated with each of the individual reactions shown in FIGURE 4, we have

$$\begin{aligned}
 [\text{Reaction}] &= V \cdot \frac{dS_{NO_3}}{dt} \Big|_{\text{Denitrification}} + V \cdot \frac{dX_A}{dt} \Big|_{\text{Growth}} \\
 &= V \left( \frac{dS_{NO_3}}{dt} \Big|_{\text{Denitrification}} + \frac{dX_A}{dt} \Big|_{\text{Growth}} \right) \\
 &= V \left[ -0.233 \frac{dX_H}{dt} \Big|_{\text{Anoxic Growth}} + \mu_{m,A} \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_{O^H} + S_0} \right) X_A \right] \\
 &= V \left[ -0.233 (0.8) X_H \left( \frac{S_s}{K_{ss} + S_s} \right) \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{K_{O^H}}{K_{O^H} + S_0} \right) + \mu_{m,A} X_A \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_{O^A} + S_0} \right) \right] \quad (8)
 \end{aligned}$$

Substituting equation (8) into equation (7) results in the following

$$0 = Q(S_{NO_3,0} - S_{NO_3}) + V \left[ -0.1864 X_H \left( \frac{S_s}{K_{ss} + S_s} \right) \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{K_{O^H}}{K_{O^H} + S_0} \right) + \mu_{m,A} X_A \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_{O^A} + S_0} \right) \right]$$

Dividing both sides of the above equation by V yields

$$0 = \cancel{\frac{Q}{V}} (S_{NO_3,0} - S_{NO_3}) - 0.1864 X_H \left( \frac{S_s}{K_{ss} + S_s} \right) \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{K_{O^H}}{K_{O^H} + S_0} \right) + \mu_{m,A} X_A \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_{O^A} + S_0} \right)$$

$$0 = \frac{1}{\theta} S_{NO_3,0} - \frac{1}{\theta} S_{NO_3} - 0.1864 X_H \left( \frac{S_s}{K_{ss} + S_s} \right) \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{K_{O^H}}{K_{O^H} + S_0} \right) + \mu_{m,A} X_A \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_{O^A} + S_0} \right)$$

$$S_{NO_3} \left[ \frac{1}{\theta} + 0.1864 X_H \left( \frac{S_s}{K_{ss} + S_s} \right) \left( \frac{1}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{K_{O^H}}{K_{O^H} + S_0} \right) \right] = \frac{1}{\theta} S_{NO_3,0} + \mu_{m,A} X_A \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_{O^A} + S_0} \right).$$

Therefore, we have that

$$S_{NO_3} = \frac{\frac{1}{\theta} S_{NO_3,0} + \mu_{m,A} X_A \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_{O^A} + S_0} \right)}{\frac{1}{\theta} + 0.1864 X_H \left( \frac{S_s}{K_{ss} + S_s} \right) \left( \frac{1}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{K_{O^H}}{K_{O^H} + S_0} \right)} \times \frac{\theta}{\theta}$$

$$S_{NO_3} = \frac{S_{NO_3,0} + \theta \left[ \mu_{m,A} X_A \left( \frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left( \frac{S_0}{K_{O^A} + S_0} \right) \right]}{1 + \theta \left[ 0.1864 X_H \left( \frac{S_s}{K_{ss} + S_s} \right) \left( \frac{1}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{K_{O^H}}{K_{O^H} + S_0} \right) \right]}$$

$$(i) \quad [\text{Change}] = [\text{Inlet}] - [\text{Outlet}] + [\text{REACTION}]$$

$$\frac{V \cdot dS_{NH}}{dt} = Q(S_{NH,0} - S_{NH}) + [\text{REACTION}] \quad \leftarrow \begin{array}{l} \text{Assumption: steady state, no separation} \\ \text{of soluble components in} \\ \text{secondary clarifier.} \end{array}$$

O (s.s)

$$0 = Q(S_{NH,0} - S_{NH}) + [\text{REACTION}].$$

$$(ii) \quad [\text{REACTION}] = V \left[ -i_{in,new} \left[ \frac{dX_H}{dt} \Big|_{\substack{\text{aerobic} \\ \text{growth}}} + \frac{dX_H}{dt} \Big|_{\substack{\text{anoxic} \\ \text{growth}}} + \frac{dX_A}{dt} \Big|_{\text{growth}} \right] + \left( \frac{X_{NS}}{X_S} \right) \left( \frac{dX_S}{dt} \Big|_{\text{hydrolysis}} \right) \right]$$

$$- \frac{1}{Y_A} \frac{dX_A}{dt} \Big|_{\text{growth}}$$

$$= V \left[ -i_{in,new} \left\{ \left[ \mu_{m,H} X_H \left( \frac{S_S}{K_{SS} + S_S} \right) \left( \frac{1}{K_{O^H} + S_O} \right) \left[ S_O + \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{1}{K_{O^H} + S_O} \right) (0.8) \right] + \right. \right. \right. \right.$$

$$\left. \left. \left. \left. \mu_{m,A} \left( \frac{S_{NH}}{S_{NH} + K_{NH}} \right) \left( \frac{S_O}{K_{O^A} + S_O} \right) X_A \right\} - X_{NS} K_h X_H - \frac{1}{Y_A} \mu_{m,A} \left( \frac{S_{NH}}{S_{NH} + K_{NH}} \right) \left( \frac{S_O}{S_O + K_{O^A}} \right) X_A \right] \right]$$

$$(iii) \quad 0 = \frac{Q}{V} (S_{NH,0} - S_{NH}) - i_{in,new} \left\{ \left[ \mu_{m,H} X_H \left( \frac{S_S}{K_{SS} + S_S} \right) \left( \frac{1}{K_{O^H} + S_O} \right) \left[ S_O + \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{1}{K_{O^H} + S_O} \right) (0.8) \right] \right. \right. \right.$$

$$\left. \left. \left. + \mu_{m,A} \left( \frac{S_{NH}}{S_{NH} + K_{NH}} \right) \left( \frac{S_O}{K_{O^A} + S_O} \right) X_A \right\} - X_{NS} K_h X_H - \frac{1}{Y_A} \mu_{m,A} \left( \frac{S_{NH}}{S_{NH} + K_{NH}} \right) \left( \frac{S_O}{S_O + K_{O^A}} \right) X_A \right]$$

$$\Rightarrow \boxed{S_{NH} = \frac{1}{\theta} S_{NH,0} - X_{NS} K_h X_H - i_{in,new} \left\{ \mu_{m,H} X_H \left( \frac{S_S}{K_{SS} + S_S} \right) \left( \frac{1}{K_{O^H} + S_O} \right) \left( \frac{S_{NO_3}}{S_{NO_3} + K_{NO_3}} \right) \left( \frac{1}{K_{O^H} + S_O} \right) (0.8) \right\}}$$

$$\boxed{\left. \left\{ \frac{1}{\theta} + i_{in,new} \mu_{m,A} \left( \frac{1}{S_{NH} + K_{NH}} \right) \left( \frac{S_O}{K_{O^A} + S_O} \right) X_A + \frac{1}{Y_A} \mu_{m,A} \left( \frac{1}{S_{NH} + K_{NH}} \right) \left( \frac{S_O}{S_O + K_{O^A}} \right) X_A \right\} \right)}$$

$$X_H = \frac{1}{\theta} X_{H,0} + \mu_m H \left( \frac{S_s}{K_{ss} + S_s} \right) \left( \frac{S_0}{S_0 + K_{O^{\prime\prime}}} \right) X_H + \mu_m H \left( \frac{S_s}{K_{ss} + S_s} \right) \left( \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) \left( \frac{K_O^H}{K_O^H + S_0} \right) 0.8 X_H$$

$$\frac{1}{\theta_c} + b_H$$

↳ Derived using the same assumptions as the other particulate components + unique reactions term based off the reaction chart.