A Fundamental Mathematical Model of a Microbial Predenitrification System

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Space flight beyond Low Earth Orbit requires sophisticated systems to support all aspects of the mission (life support, real-time communications, etc.). A common concern that cuts across all these systems is the selection of information technology (IT) methodology, software and hardware architectures to provide robust monitoring, diagnosis, and control support. Another dimension of the problem space is that different systems must be integrated seamlessly so that communication speed and data handling appear as a continuum (un-interrupted). One such team investigating this problem is the Advanced Integration Matrix (AIM) team whose role is to define the critical requirements expected of software and hardware to support an integrated approach to the command and control of Advanced Life Support (ALS) for future long-duration human space missions, including permanent human presence on the Moon and Mars. A goal of the AIM team is to set the foundation for testing criteria that will assist in specifying tasks, control schemes and test scenarios to validate and verify systems capabilities.

This project is to contribute to the goals of the AIM team by assisting with controls planning for ALS. Control for ALS is an enormous problem it involves air revitalization, water recovery, food production, solids processing and crew. In more general terms, these systems can be characterized as involving both continuous and discrete processes, dynamic interactions among the sub-systems, nonlinear behavior due to the complex operations, and a large number of multivariable interactions due to the dimension of the state space. It is imperative that a baseline approach from which to measure performance is established especially when the expectation for the control system is complete autonomous control.

ACKNOWLEDGEMENTS

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1. INTRODUCTION

The objective of the project is to treat grey water using a microbial based wastewater treatment system. Grey water is any water that has been used in the home, except water from toilets. This may include dish, shower, sink, and laundry water. This type of “water” may be reused for other purposes, especially landscape irrigation. In space studies: grey water will contain, 10% urine, hygiene (hand, shower, and oral waters), laundry water (high surfactant concentrations).

True nitrifying bacteria are considered to be those belonging to the family *nitrobacteraceae*. These bacteria are strictly aerobic, gram-negative, chemolithic autotrophs. They require oxygen, utilize mostly inorganic (without carbon) compounds as their energy source, and require carbon dioxide (CO\_2) for their source of carbon. In the case of the *nitrobacteraceae* these energy sources are derived from the chemical conversion of ammonia (NH\_4\textsuperscript+-N) to nitrite (NO\textsubscript{2}\textsuperscript{-}-N) or, nitrite (NO\textsubscript{2}\textsuperscript{-}-N) to nitrate (NO\textsubscript{3}\textsuperscript{-}-N).

*Nitrosomonas* is the most common ammonia-oxidizer while *nitrobacter* is the most common nitrite-oxidizer.

The nitrifying reactor studied contains three types of microorganisms: aerobic heterotrophs, *nitrosomonas* and *nitrobacters*. Assume that the cell can be represented generically by the formula C\textsubscript{3}H\textsubscript{7}O\textsubscript{2}N (mw=113g/gmol) and that the organic carbon donor has the formula C\textsubscript{10}H\textsubscript{19}O\textsubscript{3}N (mw= 201g/gmol).

*Nitrosomonas* oxidize the ammonium-ion to nitrite and *nitrobacters* oxidize the nitrite to nitrate. Overall

$$\frac{1}{8} NH_4^+ + \frac{3}{8} H_2O \rightarrow \frac{1}{8} NO_3^- + \frac{5}{4} H^+ + e^-$$ \hspace{1cm} (1)

These two species work together to achieve the overall oxidation of ammonium to nitrate. The nitrate is recycled to the denitrifying reactor where it is used by the microorganisms (*pseudomonas*) under anoxic conditions.

Denitrifiers are chemotrophs that use organic and inorganic electron donors. Common gram-negative denitrifiers are *Proteobacteria* such as *pseudomonas*. All denitrifiers are facultative microbes, which means they shift to either nitrate or nitrite ion respiration when oxygen is limited. Organic carbon users are heterotrophs. Denitrification proceeds in a stepwise manner:

$$\frac{1}{2} NO_3^- + e^- + H^+ \rightarrow \frac{1}{2} NO_2^- + \frac{1}{2} H_2O : \text{nitrate reduction}$$

$$NO_2^- + e^- + 2H^+ \rightarrow NO + H_2O : \text{nitrite reduction}$$

$$NO + e^- + H^+ \rightarrow \frac{1}{2} N_2O + \frac{1}{2} H_2O : \text{nitric oxide reduction}$$

$$\frac{1}{2} N_2O + e^- + H^+ \rightarrow \frac{1}{2} N_2(g) + \frac{1}{2} H_2O : \text{nitrous oxide reduction}$$
Electrons provided by the donor are used for energy (R_e) and cell synthesis (R_s),

\[ R = f_e R_e + f_s R_s \]

\[ R_e = R_a - R_d \]

\[ R_s = R_c - R_a \]

(2)

where \( R_d \) is the donor reaction, \( R_a \) is the electron acceptor reaction, and \( R_c \) is the cell synthesis reaction. The relationship between \( f_e \), fraction used for energy, and the fraction used for cell synthesis is \( f_s = 1 - f_e \).

2. PREDENITRIFICATION SYSTEM

Consider the following two reactors in series and a settler, shown in Figure 1. The first reactor is a denitrifier that converts organic carbon compounds under anoxic conditions (absence of oxygen) for energy and nitrate-ion (electron acceptor) for cellular respiration. Carbon dioxide and a source of nitrogen (ammonium-ion) are used for cell synthesis. Other nutrients such as phosphorous should also be supplied. The second reactor is the nitrifier that operates aerobically and consists of nitrosomonas, nitrobacters, and aerobic heterotrophs. Oxygen is used for cellular respiration and is supplied in the form of air (79% \( \text{N}_2 \), 21% \( \text{O}_2 \)). Any organic carbons unused by the pseudomonas are the source of energy for the aerobic heterotrophs. Ammonium-ion: \( (\text{NH}_4^+ - N) \) is used by nitrosomonas for energy (produce nitrite-ion \( (\text{NO}_2^- - N) \)) and both nitrosomonas and nitrobacters also use the ammonium-ion for cell synthesis. The nitrite-ion is used (reduced) by the nitrobacters for energy. The product, the nitrate-ion \( (\text{NO}_3^- - N) \) is recycled to the denitrifier for cellular respiration. The rate of cell synthesis in the denitrifier is limited by the supply of nitrate-ion. The recommended recycle rate is 4 to 6 times the influent stream to the denitrifier.

\[ f_d = \frac{1}{1 + b \theta_x} \left( \frac{f_s}{f_s^0} (1 + b \theta_x) - 1 \right) \]

\[ f_s = \frac{f_s^0 (1 + (1 - f_d) b \theta_x)}{1 + b \theta_x} \]

(3)
2.1 STOICHIOMETRY

2.1.1 DENITRIFIER (ANOXIC REACTOR)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Pseudomonas</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f^0$</td>
<td>0.52</td>
</tr>
<tr>
<td>$Y$ mgVSSa/mgBOD$_L$</td>
<td>0.26</td>
</tr>
<tr>
<td>$\dot{q}$ mgBOD$_L$/mgVSSa-d</td>
<td>12</td>
</tr>
<tr>
<td>$\dot{q}$ mgNO$_2$/mgVSSa-d</td>
<td>16</td>
</tr>
<tr>
<td>$K$ mgBOD$_L$/L</td>
<td>10</td>
</tr>
<tr>
<td>$K_{\text{max}}$ mgNO$_2$/L</td>
<td>10</td>
</tr>
<tr>
<td>$\theta$ d</td>
<td>5</td>
</tr>
<tr>
<td>$b$ d</td>
<td>0.052</td>
</tr>
<tr>
<td>$\theta^\text{min}$ d</td>
<td>0.33</td>
</tr>
<tr>
<td>$S_{\text{min}}$ mgNO$_2$/L</td>
<td>0.017</td>
</tr>
<tr>
<td>$f_4$</td>
<td>0.8</td>
</tr>
<tr>
<td>$f_5$</td>
<td>0.4342</td>
</tr>
</tbody>
</table>

Table 1: Typical parameters for a Denitrifier: $T=20^\circ$C (Rittman and McCarty)

**Pseudomonas**

$$R_a: \frac{1}{5} \text{NO}_2^- + \frac{6}{5} \text{H}^+ \rightarrow \frac{1}{10} \text{N}_2 + \frac{3}{5} \text{H}_2 \text{O}$$

$$R_c: \frac{1}{5} \text{CO}_2 + \frac{1}{20} \text{HCO}_3^- + \frac{1}{20} \text{NH}_4^+ + \text{H}^+ \rightarrow \frac{1}{50} \text{CO}_2 + \frac{1}{50} \text{HCO}_3^- + \frac{1}{50} \text{NH}_4^+ + \text{H}^+$$

$$R_d: \frac{1}{50} \text{CO}_2 + \frac{1}{19} \text{H}_2 \text{O} \rightarrow \frac{9}{25} \text{CO}_2 + \frac{1}{50} \text{HCO}_3^- + \frac{1}{50} \text{NH}_4^+ + \text{H}^+$$

2.2 NITRIFIER (AEROBIC REACTOR):

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Nitrosomonas</th>
<th>Nitrobacters</th>
<th>Aerobic Heterotrophs</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f^0$</td>
<td>0.14</td>
<td>0.10</td>
<td>0.7</td>
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<tr>
<td>$Y$ mgVSSa/mgNH$_4$</td>
<td>0.33</td>
<td>0.083 mgVSSa/mgNO$_2$</td>
<td>0.45 mgVSSa/mgBOD$_L$</td>
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<tr>
<td>$\dot{q}$ mgNO$_2$/mgVSSa-d</td>
<td>1.7 mgNH$_3$/mgVSSa-d</td>
<td>7.3 mgNO$_2$/mgVSSa-d</td>
<td>10 mgBOD$_L$/mgVSSa-d</td>
</tr>
<tr>
<td>$K$</td>
<td>0.57 mgNH$_4$/L</td>
<td>0.62 mgNO$_2$/L</td>
<td>10 mgBOD$_L$/L</td>
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<tr>
<td>$K_{\text{max}}$ mgNO$_2$/L</td>
<td>0.5</td>
<td>0.68</td>
<td>0.1</td>
</tr>
<tr>
<td>$b$ d</td>
<td>0.082</td>
<td>0.082</td>
<td>0.1</td>
</tr>
<tr>
<td>$f^\text{lim}_x$</td>
<td>2.1</td>
<td>1.9</td>
<td></td>
</tr>
<tr>
<td>$S_{\text{min,ox}}$ mgO$_2$/L</td>
<td>0.084</td>
<td>0.12</td>
<td></td>
</tr>
<tr>
<td>$S_{\text{min,N}}$</td>
<td>0.094 mgNH$_4$/L</td>
<td>0.1 mgNO$_2$/L</td>
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<tr>
<td>$f_4$</td>
<td>0.067</td>
<td>0.067</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Table 2: Typical parameters for a Nitrifier: $T=15^\circ$C (Table 9.1, p 472, Rittman and McCarty)
**Nitrosomonas**

\[
R_a: \frac{1}{4} O_2 + H^+ + e^- \rightarrow \frac{1}{2} H_2 O
\]

\[
R_c: \frac{1}{5} CO_2 + \frac{1}{20} HCO^-_3 + \frac{1}{20} NH^+_4 + H^+ + e^- \rightarrow \frac{1}{20} C_5 H_7 O_2 N + \frac{9}{20} H_2 O
\]

\[
R_d: \frac{1}{6} NH^+_4 + \frac{1}{3} H_2 O + e^- \rightarrow \frac{1}{6} NO^-_2 + \frac{2}{3} H^+
\]

\[
R: \frac{(1-f_s)}{4} O_2 + \frac{f_s}{5} CO_2 + \frac{f_s}{20} HCO^-_3 + \left(\frac{1}{6} + \frac{f_s}{20}\right)NH^+_4 \rightarrow \frac{f_s}{20} C_5 H_7 O_2 N + \frac{1}{6} NO^-_2 + \left(\frac{1}{6} - \frac{f_s}{20}\right)H_2 O + \frac{1}{3} H^+
\]

**Nitrobacter**:

\[
R_a: \frac{1}{4} O_2 + H^+ \rightarrow \frac{1}{2} H_2 O
\]

\[
R_c: \frac{1}{3} CO_2 + \frac{1}{20} HCO^-_3 + \frac{1}{20} NH^+_4 + H^+ \rightarrow \frac{1}{20} C_5 H_7 O_2 N + \frac{9}{20} H_2 O
\]

\[
R_d: \frac{1}{3} NO^-_2 + \frac{1}{2} H_2 O \rightarrow \frac{1}{2} NO^-_3 + H^+
\]

\[
R: \frac{1-f_s}{4} O_2 + H^+ + \frac{f_s}{2} CO_2 + \frac{f_s}{20} HCO^-_3 + \frac{f_s}{20} NH^+_4 + \frac{1}{2} NO^-_2 \rightarrow \frac{1}{2} NO^-_3 \frac{f_s}{20} C_5 H_7 O_2 N + \frac{f_s}{20} H_2 O
\]

**Aerobic Heterotrophs**:

\[
R_a: \frac{1}{4} O_2 + H^+ \rightarrow \frac{1}{2} H_2 O
\]

\[
R_c: \frac{1}{3} CO_2 + \frac{1}{20} HCO^-_3 + \frac{1}{20} NH^+_4 + H^+ \rightarrow \frac{1}{20} C_5 H_7 O_2 N + \frac{9}{20} H_2 O
\]

\[
R_d: \frac{1}{30} C_{16} H_{19} O_2 N + \frac{2}{30} H_2 O \rightarrow \frac{2}{30} CO_2 + \frac{1}{30} HCO^-_3 + \frac{1}{30} NH^+_4 + H^+
\]

\[
R: \frac{1-f_s}{4} O_2 + \frac{1}{30} C_{16} H_{19} O_2 N + \left(\frac{f_s}{3} - \frac{2}{30}\right) CO_2 + \left(\frac{f_s}{20} - \frac{1}{30}\right) HCO^-_3 + \left(\frac{f_s}{20} - \frac{1}{30}\right) NH^+_4 \rightarrow \frac{f_s}{30} C_5 H_7 O_2 N + \left(\frac{7}{30} - \frac{f_s}{30}\right) H_2 O
\]

3. MODELING

Streams appear as subscripts; components appear as superscripts. Properties of a unit operation appear as subscripts (N: nitrifier, D: denitrifier, T: settler). For example V_N: volume of the nitrifier. The following balances are with reference to Figure 1.

3.1 DENITRIFIER

Input streams are: Q^0 (L/d), pQ_2 (L/d), v (1-p) Q_2 (L/d). Input biochemical oxygen demands (BOD_3) are the carbon source, S^0 (mg BOD_3/L), the nitrogen (total Kjedahl nitrogen or TKN) source, S_n^0 (mg N/L), the nitrate-ion, S_n (mg NO_3-N/L), and the initial amount of inerts, x_i^0 (mgVSS/L). Pseudomonas (x_p: mgVSSa/L) biomass is the active volatile suspended solids (VSSa) and x_v (mgVSS/L) = x_p + x_i is the total volatile suspended solids in the effluent.

3.1.1 COMPONENT BALANCES
biomass: \( V_D \frac{dx}{dt} = Q_0 x_p^0 + Q_2 f_d (\rho x v_2 + \nu(1 - \rho)) x_w - Q_1 x_p + (r_p P - b P x_p) V_D \)

orgC: \( V_D \frac{dS_1}{dt} = Q_0 S_0^0 + \rho Q_2 S_2^0 + \nu(1 - \rho) Q_2 S_2 - Q_1 S_1 - r_p V_D \)

NO\(_3^-\): \( V_D \frac{dS_{no1}}{dt} = \rho Q_2 S_{no2} + \nu(1 - \rho) S_{no2} - Q_1 S_{no1} - r_{no} V_D \) \( (4) \)

TKN: \( V_D \frac{dS_{nh1}}{dt} = Q_0 S_{nh}^0 + \rho Q_2 S_{nh2} + \nu(1 - \rho) Q_2 S_{nh2} - Q_1 S_{nh1} - r_{nh} V_D \)

inerts: \( V_D \frac{dx}{dt} = Q_0 x_{i2}^0 - Q_1 x_{i1} + (1 - f_d) b (x_{v2} + x_w + x_{p1}) V_D \)

utilRate: \( r_p = \frac{\dot{q} P S_1}{K P + S_1} x_p (\text{mgBOD}_L/L - d) \)

where \( Y_p \) is the true yield for synthesis; \( f_d \) is the fraction of the active biomass (\( x_p \)) and recycled volatile suspended solids that is biodegradable, \( x_i^0 \) is the influent inert concentration, \( K_P \) is that concentration that gives one-half the maximum growth rate, \( \dot{q} \) is the maximum specific rate of substrate utilization, \( b_P \) is the endogenous decay coefficient, \( \rho \) is that fraction of the effluent stream (\( Q_2 \)) of the nitrifier that is recycled to the denitrifier, \( S_{nh} \) is the ammonium-ion, \( (1 - \nu) \) is that fraction of the influent stream \( ((1 - \rho) Q_2) \) to the settler that is recycled to the denitrifier, and \( x_{v2}, x_w \) are the mixed liquor compositions that are recycled from the nitrifier and waste stream of the settler, respectively.

Define the hydraulic detention time (HDT, units of days), \( \theta_D \), in the denitrifier, and the nitrifier, \( \theta_N \), respectively by

\[ \theta_D = \frac{V_D}{Q_0} \quad \text{and} \quad \theta_N = \frac{V_N}{Q_1} \] \( (5) \)

The mean cell retention time, \( \theta_{MCRT} \), (MCRT same as solids retention time or the sludge age, units of days) is defined by

\[ \theta_{MCRT} = \frac{V \cdot \text{active biomass}}{Q_1 \cdot \text{produced biomass}} \] \( (6) \)

A useful relationship between the MCRT and the HRT is given by

\[ \theta = \frac{\theta_s}{w_v} \left( \Delta(V x_v) \right) = \lim_{t \to 0} \frac{\theta_s}{w_v} \left( \frac{d(V x_v)}{dt} \right) = \frac{\theta_s}{w_v} (Q_1 x_v) \] \( (7) \)
where $w_v$ (mgVSS/L) is the mixed-liquor volatile suspended solids (MLVSS or holdup) and $Q$, $x_v$ is the mass production rate of the total VSS (active, inerts, soluble microbial products (SMP)).

3.1.2 ASSUMPTIONS
1. There is no active biomass in the input stream, thus $x_p = 0$.
2. There are no TKN and organic carbons present in the effluent stream of the nitrifier.
   Thus, $S_{nh2} = 0$, $S_{o2} = 0$.
3. There is no nitrate-ion in the effluent stream of the settler, thus $S_{noe} = 0$ but $S_{no} = S_{no2}$.
4. Only $f_d$ of the mixed liquor ($x_{v2}, x_w$) returned to the denitrifier in either recycle streams is active biomass.

Applying the assumptions and simplifying the system of equations in (4) give,

$$\frac{dx_{p1}}{dt} = \frac{Q_2}{V_D} f_d (p x_{v2} + v (1 - p) x_w) - \frac{Q_1}{V_D} x_p + (Y_pr_p - b_p x_p)$$

$$\frac{dS_i}{dt} = S_0 - \frac{Q_1}{V_D} S_i - r_p$$

$$\frac{dS_{no1}}{dt} = \frac{Q_2}{V_D} (p + v (1 - p) S_{no2} - \frac{Q_1}{V_D} S_{no1} - r_{no})$$

$$\frac{dS_{nh1}}{dt} = S_0 - \frac{Q_1}{V_D} S_{nh1} - r_{nh}$$

$$\frac{dx_{i1}}{dt} = \frac{x_i^0}{\theta_D} - \frac{Q_1}{V_D} x_{i1} + (1 - f_d) b (x_{v2} + x_w + x_p)$$

Design variables are recycle fractions ($\rho$, $v$), mean cell retention time, $\theta_D$, MLVSS, $w_v D, Q_l, Q^0$. Reasonable choices of $\rho (1 - v) (1 - \rho)$ are 6 and 0.25, respectively. In the case of HDT and MCRT, good choices are 0.75 and 15 days, respectively.

REMARKS
1. Nitrogen balance on the nitrifier will indicate the amount of nitrate-ion ($S_{no2}$) in stream 2 (effluent from nitrifier) that is an input stream to the denitrifier. Define

$$\gamma = \frac{14 \text{ mgN}}{113 \text{ mgVSS}}$$

that represents the mass of nitrogen present in the biomass. A steady-state component balance on the nitrate-ion in the effluent of the reactor is given by,

$$Q_2 S_{no2} (\text{mgNO3/d}) = Q^0 S_i - \left(Q_1 x_{i1}^o + Q_2 x_{i2}^o\right) \gamma$$

$$x_{i1}^o = x_{p1} + x_{i1} - x_i^o$$

$$x_{i2}^o = x_{H2} + x_{N2} + x_{i2} - x_i^o$$

The dynamic balance is given by,
\[
V_n \frac{dS_{no2}}{dt} = Q_s^0 S_{n1} - Q_{1} x_{sD} \gamma - Q_{2} S_{no2} - (r_{h} - r_{n}) V_n
\]  

(11)

In the dynamic balance equation, \( r_{n} \) and \( r_{h} \) are the utilization rates of the nitrate-ion by the nitrifiers and the aerobic heterotrophs.

2. The steady-state value of the ammonium-ion is a function of amount of organic substrate consumed. By stoichiometry,

\[
\overline{S_{nh1}} = \frac{\left(\frac{f}{20} - \frac{1}{50}\right)}{50} \left(\frac{14 \text{ mgN}}{201 \text{ mgBOD}}\right) \text{ (substrate consumption rate)}
\]  

(12)

3. The utilization, \( r_{h} \), of the organic substrate, \( C_{10}H_{19}O_{2}N \), by the aerobic heterotroph is based on the amount of nitrate-ion present. Thus, the nitrate-ion is the limiting component.

The total sludge leaving the denitrifier is given by:

\[
\frac{\Delta (V_d x_{sD})}{\Delta t} \text{ (mgVSS/d)} = Q_{1} x_{r} = \frac{w_{r} Q_{0}^{0} \theta_{D}}{\theta_{xD}} = \frac{w_{r} V_{D}}{\theta_{xD}}
\]  

(13)

3.1.3 STEADY STATE

The steady state of the denitrifier (variables with an overbar) is given by,

\[
\begin{align*}
\bar{x}_{p1} &= \left(\frac{Q_{2}}{V_{D}} f_{d} (\rho_{v2} + (1 - \nu)(1 - \rho))\bar{x}_{w} - y_{p} (\frac{s_{v}}{\theta_{D}} - \frac{Q_{1} \bar{x}_{1}}{Q_{1}}) \frac{V_{D}}{\theta_{D}} \right) \frac{V_{D}}{\theta_{D}} - \frac{Q_{0} s_{v}}{Q_{1} \theta_{D}} K_{P} - \frac{Q_{0} s_{v}}{Q_{1} \theta_{D}} \\
\bar{s}_{1} &= \frac{- (\frac{Q_{0} s_{v}}{Q_{1} \theta_{D}} - K_{P} - \bar{x}_{p1}) V_{D}}{2} \frac{V_{D}}{\theta_{D}} - \frac{Q_{0} s_{v}}{Q_{1} \theta_{D}} K_{P} - \frac{Q_{0} s_{v}}{Q_{1} \theta_{D}} \\
\bar{s}_{no1} &= \frac{- (\frac{Q_{2} S_{no2}}{Q_{1} \theta_{D}} - K_{no} - \bar{x}_{no1}) V_{D}}{2} \frac{V_{D}}{\theta_{D}} - \frac{Q_{2} S_{no2}}{Q_{1} \theta_{D}} K_{no} - \frac{Q_{2} S_{no2}}{Q_{1} \theta_{D}} \\
\bar{s}_{nh1} &= \frac{- (\frac{Q_{0} s_{v}}{Q_{1} \theta_{D}} - K_{nh} - \bar{x}_{nh1}) V_{D}}{2} \frac{V_{D}}{\theta_{D}} - \frac{Q_{0} s_{v}}{Q_{1} \theta_{D}} K_{nh} - \frac{Q_{0} s_{v}}{Q_{1} \theta_{D}} \\
\bar{x}_{II} &= \frac{V_{D}}{Q_{1} \theta_{D}} \left( \frac{\bar{x}_{v2}}{V_{D}} + (1 - f_{d}) b_{P} (\bar{x}_{v2} + \bar{x}_{vw} + \bar{x}_{p1}) \right)
\end{align*}
\]  

(14)
3.2 NITRIFIER
Nitrogen supply to the nitrifier starts as effluent TKN from the denitrifier (amount not used by the pseudomonas). TKN hydrolyzes to ammonium, $NH_4^+ - N$, and nitrite, $NO_2^- - N$. Ammonium is used in the nitrifier by all microorganisms, heterotrophs, nitrosomonas and nitrobacters for cell synthesis; but nitrosomonas also uses ammonium for energy while nitrobacters uses nitrite for energy. $NH_4^+ - N (S_{nh})$ is the limiting substrate for nitrosomonas, $NO_2^- - N (S_{no})$ is the limiting substrate for nitrobacters. The amount of TKN nitrogen available for nitrobacters is a function of the amount that is unused by the heterotrophs, nitrosomonas and any inerts (or SMP).

Heterotrophs: $x_H$, Nitrosomonas: $x_s$, Nitrobacters: $x_B$, organic carbon: $S$

3.2.1 COMPONENT BALANCES

$$V_N \frac{dx_H}{dt} = Q_H x_H^0 - Q_2 x_{H2} + (V_H r_H - b_H x_{H2}) V_N$$

$$V_N \frac{dS}{dt} = Q_1 S_1 - Q_2 S_2 - r_H V_N$$

$$V_N \frac{dx_s}{dt} = Q_1 x_s - Q_2 x_{s2} + (V_s r_s - b_s x_s) V_N$$

$$V_N \frac{dS_{nh}}{dt} = Q_1 S_{nh1} - Q_2 S_{nh2} - V_N r_s$$

$$V_N \frac{dx_B}{dt} = Q_1 x_B - Q_2 x_{B2} + (V_B r_B - b_B x_{B2}) V_N$$

$$V_N \frac{dS_{no}}{dt} = Q_1 S_n - Q_2 S_{no2} - V_N r_B$$

$$V_N \frac{dx}{dt} = Q_0 x^0_0 - Q_2 x_{12} + (1 - f_a) (b_H x_{H2} + b_N x_{N2} + b_B x_{B2}) V_N$$

The utilization terms $r_H$, $r_s$, and $r_B$ are given by:

$$r_H = \frac{\hat{q}_H S_2}{K_H + S_2} x_{H2}$$

$$r_s = \frac{\hat{q}_s S_{nh2}}{K_s + S_{nh2}} x_s$$

$$r_B = \frac{\hat{q}_B S_{no2}}{K_B + S_{no2}} x_{B2}$$

The total sludge leaving the denitrifier is given by:

$$\frac{\Delta (V_N x_N)}{\Delta t} (mg VSS/d) = Q_2 x_v = \frac{w_{vn} Q_1 \theta_N}{\theta_{x_N}} = \frac{w_v V_N}{\theta_{x_N}}$$
The difference between the influent nitrogen and the amount of biomass (heterotrophs and nitrosomonas and the biodegradable inerts) produced indicates how much nitrate-ion remains for cell maintenance of the nitrobacters.

\[
V_N \frac{dS_{no2}}{dt} = Q_L \left( S_{n1} - \frac{\theta_N}{\theta_{SN}} (\bar{x}_H + \bar{x}_S + \bar{x}_I) \right) - Q_2 S_{no2} - V_N r_B \tag{18}
\]

The amount of unused nitrogen is given by

\[
\bar{S}_{n2} = \bar{S}_{n1} - \frac{\theta_N}{\theta_{SN}} (\bar{x}_a + \bar{x}_s + \bar{x}_b + \bar{x}_I) y - \bar{S}_{nh1} - \bar{S}_{no2} \tag{19}
\]

3.2.2 STEADY STATE

At steady state, the above equations can be solved to give,

\[
\bar{x}_H = \frac{\theta_N}{\theta_{SN}} \left( \frac{\bar{S}_1 - \bar{S}_2}{1 + b_H \theta_{SN}} \right) Y_H
\]

\[
\bar{S}_2 = \frac{K_H (1 + b_H \theta_{SN})}{\theta_{SN} (Y_H \bar{q}_H - b_H)} - 1
\]

\[
\bar{x}_S = \frac{\theta_{SN}}{\theta_N} \left( \frac{S_{nh1} - \bar{S}_{nh2}}{1 + b_S \theta_{SN}} \right) Y_S
\]

\[
\bar{S}_{nh2} = K_S \left( \frac{1 + b_S \theta_{SN}}{\theta_{SN} (Y_S \bar{q}_S - b_S)} \right) - 1
\]

\[
\bar{x}_B = \frac{\theta_{SN}}{\theta_N} \left( \frac{\bar{S}_{no21} - \bar{S}_{no22}}{1 + b_B \theta_{SN}} \right) Y_B
\]

\[
\bar{S}_{no2} = K_B \left( \frac{1 + b_B \theta_{SN}}{\theta_{SN} (Y_B \bar{q}_B - b_B)} \right) - 1
\]

\[
\bar{x}_{i2} = \frac{\theta_{SN}}{\theta_N} \left( \bar{x}_{ni} + \theta_N (1 - f_d) (b_H \bar{x}_H + b_S \bar{x}_S + b_B \bar{x}_B) \right)
\]

3.3 SETTLER

Because a net growth of microorganisms is obtained, the net growth called excess sludge or waste sludge is removed from the system for subsequent sludge treatment and disposal. It is crucial that the quantity of waste sludge (bio-solids) produced must be removed continually in order to maintain the steady-state conditions. The rate of sludge wasting is essential for operating the treatment system and for determining the total cost of construction and operation of the system.

3.3.1 MATERIAL AND COMPONENT BALANCES
\[
\frac{dV_T}{dt} = (1 - \rho)Q_e - (Q_e + Q_w) - (1 - \nu)(1 - \rho)Q_2
\]

\[
V_T \frac{dS_{NO2_e}}{dt} = (1 - \rho)Q_2S_{NO2_e} - (Q_e + Q_w + (1 - \nu)(1 - \rho)Q_2)S_{NO2_e}
\]

(21)

\[
V_T \frac{dx_{vw}}{dt} = (1 - \rho)Q_2x_{v2} - (Q_e + (1 - \nu)(1 - \rho)Q_2)x_{vw}
\]

3.3.2 ASSUMPTIONS
1. No unused organic carbon substrate or nitrogen (in the form of ammonium-ion or nitrite-ion).
2. The concentration of nitrate-ion is the same in the waste, recycle, and effluent streams.
3. The concentration of biomass is the same in the recycle and waste streams with no biomass losses in the effluent stream.

3.3.3 STEADY STATE
\[
Q_e + Q_w = \nu(1 - \rho)Q_2
\]

\[
S_{NO2_e} = S_{NO2_e}
\]

\[
x_{vw} = \frac{(1 - \rho)}{(1 - \nu)(1 - \rho)Q_2 + Q_w}Q_2
\]

(22)

4. SUMMARY
Models of the prednitrifying system were developed in the Mathworks (Natick, MA) Matlab® and simulated to study parameter sensitivities and design considerations.
**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>BAP</td>
<td>Biomass associated products</td>
</tr>
<tr>
<td>BOD</td>
<td>Biochemical oxygen demand</td>
</tr>
<tr>
<td>COD</td>
<td>Chemical oxygen demand</td>
</tr>
<tr>
<td>C_{10}H_{19}O_{3}N</td>
<td>Organic carbon substrate</td>
</tr>
<tr>
<td>C_{3}H_{2}O_{2}N</td>
<td>Cell or biomass empirical formula</td>
</tr>
<tr>
<td>HDT</td>
<td>Hydraulic detention time</td>
</tr>
<tr>
<td>MCRT</td>
<td>Mean cell retention time</td>
</tr>
<tr>
<td>MLVSS</td>
<td>Mixed liquor volatile suspended solids, mgVSS/L</td>
</tr>
<tr>
<td>OD</td>
<td>Oxygen demand (oxygen equivalents)</td>
</tr>
<tr>
<td>SMP</td>
<td>Soluble microbial products</td>
</tr>
<tr>
<td>SRT</td>
<td>Solids retention time</td>
</tr>
<tr>
<td>TKN</td>
<td>Total Kjeldahl nitrogen</td>
</tr>
<tr>
<td>UAP</td>
<td>Utilization associated products</td>
</tr>
<tr>
<td>VSS,VSSa</td>
<td>Volatile suspended solids, active volatile suspended solids</td>
</tr>
<tr>
<td>b</td>
<td>Endogenous rate of decay coefficient, 1/d</td>
</tr>
<tr>
<td>d</td>
<td>Day</td>
</tr>
<tr>
<td>f_{e}</td>
<td>Fraction of electrons used for energy</td>
</tr>
<tr>
<td>f_{d}</td>
<td>Fraction of active biomass that is biodegradable</td>
</tr>
<tr>
<td>f_{s}</td>
<td>Fraction of electrons used for synthesis</td>
</tr>
<tr>
<td>f_{s}^{0}</td>
<td>Total number of electrons transferred to the electron acceptor</td>
</tr>
<tr>
<td>r_{k}</td>
<td>Rate of utilization by biomass component K (K=B,H,P,S)</td>
</tr>
<tr>
<td>K</td>
<td>Substrate concentration that give ½ the maximum rate, mgBOD/L</td>
</tr>
<tr>
<td>\dot{q}</td>
<td>Maximum specific rate of substrate utilization, mgBOD/mgVSS-d</td>
</tr>
<tr>
<td>Q_{0}</td>
<td>Inlet volumetric feed rate, L/d</td>
</tr>
<tr>
<td>Q_{j}</td>
<td>Volumetric rate of stream j, L/d</td>
</tr>
<tr>
<td>r</td>
<td>Rate of substrate utilization, mgBOD/L-d</td>
</tr>
<tr>
<td>R_{e}</td>
<td>Energy reaction</td>
</tr>
<tr>
<td>R_{d}</td>
<td>Donor reaction</td>
</tr>
<tr>
<td>R_{s}</td>
<td>Cell synthesis reaction</td>
</tr>
<tr>
<td>S_{0}</td>
<td>Organic substrate influent concentration, mgBOD/L</td>
</tr>
<tr>
<td>S_{i}</td>
<td>Substrate concentration in stream j, mgBOD/L</td>
</tr>
<tr>
<td>S_{NO3}</td>
<td>Nitrate-ion concentration, mgNO3-N/L</td>
</tr>
<tr>
<td>S_{NO2}</td>
<td>Nitrite-ion concentration, mgNO2-N/L</td>
</tr>
<tr>
<td>S_{NH4}</td>
<td>Ammonium concentration, mgNH4-N/L</td>
</tr>
<tr>
<td>S_{NH3}</td>
<td>Influent nitrogen concentration, mgN/L</td>
</tr>
<tr>
<td>x_{ki}</td>
<td>k^{th} biomass component in stream j, mgVSS/L</td>
</tr>
<tr>
<td>x_{i}</td>
<td>Influent inert concentration, mgVSS/L</td>
</tr>
<tr>
<td>x_{ij}</td>
<td>Active volatile suspended solids in stream j, mgVSS/L</td>
</tr>
<tr>
<td>x_{i}</td>
<td>Non-biodegradable portion of the biomass, mgVSS/L</td>
</tr>
<tr>
<td>x_{B}</td>
<td>Concentration of biomass associated products, mgBOD/L</td>
</tr>
<tr>
<td>x_{U}</td>
<td>Concentration of utilized associated products, mgBOD/L</td>
</tr>
<tr>
<td>V_{D}, V_{N}, V_{T}</td>
<td>Denitrifier volume, nitrifier volume, settler volume, L/d</td>
</tr>
</tbody>
</table>
\( Y \)  
True cell synthesis yield, mgVSS/mgBOD\(_L\)

\( Y_n \)  
Net yield, mgVSS/mgBOD\(_L\)

**GREEK LETTERS**

\( \rho \)  
Fraction of effluent of nitrifier that is recycled to the denitrifier

\( (1-\nu) \)  
Fraction of influent to the settler that is recycled to the denitrifier

\( \gamma \)  
Ratio of \( \frac{1}{2} \) molecular weight of nitrogen to that of biomass

\( \theta_D, \theta_N \)  
Hydraulic detention time (HDT) in denitrifier and nitrifier, d

\( \theta_x \)  
Mean cell retention time (MCRT) or solids retention time (SRT), d

\( \theta_{x,\text{min}} \)  
Min MCRT) or min SRT, d

\( [\theta_{x,\text{min}}]_{\text{lim}} \)  
Lower bound on the min MCRT) or min SRT, d

**SUBSCRIPTS**

\( e \)  
Effluent of the settler

\( v \)  
Volatile suspended solids

\( w \)  
Waste stream

\( B \)  
*Nitrobacters*, biomass associated SMP

\( D \)  
Denitrifier

\( H \)  
Aerobic heterotrophs (nitrifier)

\( N \)  
Nitrifier

\( P \)  
*Pseudomonas*

\( S \)  
*Nitrosomonas*

\( T \)  
Settler

\( U \)  
Utilization associated SMP
REFERENCES


