A Fundamental Mathematical Model of a Microbial Predenitrification System

Final Report

NASA Faculty Fellowship Program – 2004

Johnson Space Center

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Date Submitted:	August 13, 2004
Contract Number:	NAG 9-1526 and NNJ04JF93A

ABSTRACT

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

This work was made possible not only by the financial support of the NASA's NFFP program, but also by the active participation of NASA civil servant and my collaborator David Overland (Engineering, ER2). Technical assistance and many useful discussions were provided by Marvin Ciskowski (Lockheed) and David Overland. Program outreach support was provided by Gretchen Thomas (NASA), Heather Paul (NASA), Laura Labuda (Lockheed Martin), and Debbie Berdich (Lockheed Martin).

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: gray 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 *nitro-bacteraceae*. 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^+-N) to nitrite (NO_2^--N) or, nitrite (NO_2^--N) to nitrate (NO_3^--N). *Nitrosomonas* is the most common ammonia-oxidizer while *nitrobacter* is the most common nitrite-oxidizer.

The nitrifiying reactor studied contains three types of microorganisms: aerobic heterotrophs, *nitrosomonas* and *nitrobacters*. Assume that the cell can be represented generically by the formula $C_5H_7O_2N$ (mw=113g/gmol) and that the organic carbon donor has the formula $C_{10}H_{19}O_3N$ (mw= 201g/gmol).

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

$$\tfrac{1}{8}NH_4^+ + \tfrac{3}{8}H_2O \mapsto \tfrac{1}{8}NO_3^- + \tfrac{5}{4}H^+ + e^- \qquad (1)$$

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.

Dentrifiers are chemotrophs that use organic and inorganic electron donors. Common gram-negative dentrifiers are *Proteobacteria* such as *pseudomonas*. All dentrifiers 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:

$$\tfrac{1}{2}NO_3^- + e^- + H^+ \mapsto \tfrac{1}{2}NO_2^- + \tfrac{1}{2}H_2O : \text{nitrate reduction}$$
$$NO_2^- + e^- + 2H^+ \mapsto NO + H_2O : \text{nitrite reduction}$$
$$NO + e^- + H^+ \mapsto \tfrac{1}{2}N_2O + \tfrac{1}{2}H_2O : \text{nitric oxide reduction}$$
$$\tfrac{1}{2}N_2O + e^- + H^+ \mapsto \tfrac{1}{2}N_2(g) + \tfrac{1}{2}H_2O : \text{nitrous oxide reduction}$$

Electrons provided by the donor are used for energy (R_e) and cell synthesis (R_s),

$$R = f_e R_e + f_s R_s$$
$$R_e = R_a - R_d \qquad (2)$$
$$R_s = R_c - R_d$$

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

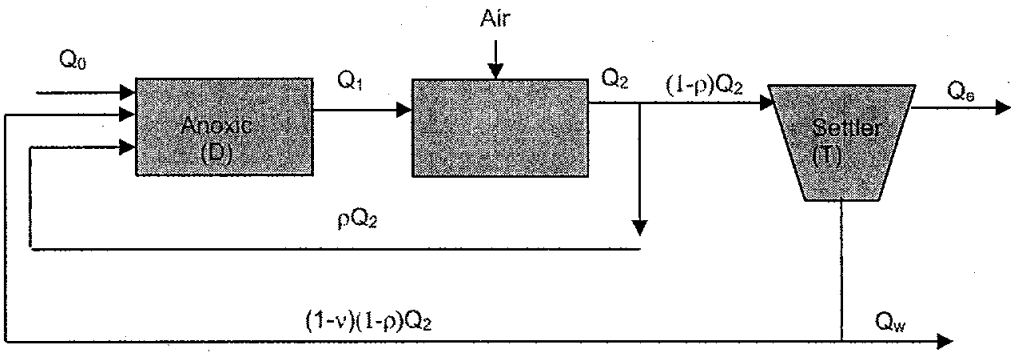

Figure 1: Denitrifier and nitrifier in series with a settler that return active sludge. The nitrifier returns a high concentration of nitrate-ion to the denitrifier.

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% N_2, 21% O_2). Any organic carbons unused by the *pseudomonas* are the source of energy for the aerobic heterotrophs. Ammonium-ion: ($NH_4^+ - N$)) is used by *nitrosomonas* for energy (produce nitrite-ion ($NO_2^- - N$)) 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 ($NO_3^- - N$)) 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.

$$f_d = 1 - \frac{1}{1+b\theta_x}\left(\frac{f_s}{f_s^0}(1+b\theta_x) - 1\right)$$
$$f_s = \frac{f_s^0\left(1+(1-f_d)b\theta_x\right)}{1+b\theta_x} \qquad (3)$$

2.1 STOICHIOMETRY

2.1.1 DENITRIFIER (ANOXIC REACTOR)

Parameter	*Pseudomonas*
f_s^0	0.52
Y mgVSSa/mgBOD$_L$	0.26
$\hat{q}$ mgBOD$_L$/mgVSSa-d	12
$\hat{q}$ mgNO$_3$/mgVSSa-d	16
K mgBOD$_L$/L	1
K_{no} mgNO3/L	10
θ_x d	5
b d	0.052
$\left[\theta_x^{min}\right]_{lim}$ d	0.33
S_{min} mgNO$_3$/L	0.017
f_d	0.8
f_s	0.4342

Table 1: Typical parameters for a Denitrifier: T=20^{0}C (Rittman and McCarty)

Pseudomonas

$$R_a : \frac{1}{5}NO_3^- + \frac{6}{5}H^+ \mapsto \frac{1}{10}N_2 + \frac{3}{5}H_2O$$

$$R_c : \frac{1}{5}CO_2 + \frac{1}{20}HCO_3^- + \frac{1}{20}NH_4^+ + H^+ \mapsto \frac{1}{20}C_5H_7O_2N + \frac{9}{20}H_2O$$

$$R_d : \frac{1}{50}C_{10}H_{19}O_3N + \frac{9}{25}H_2O \mapsto \frac{9}{50}CO_2 + \frac{1}{50}HCO_3 + \frac{1}{50}NH_4^+ + H^+$$

$$\frac{1}{50}C_{10}H_{19}O_3N + \frac{fe}{5}NO_3^- + (\frac{1}{5} - \frac{fs}{5})H^+ + (\frac{fs}{5} - \frac{9}{50})CO_2 + (\frac{fs}{20} - \frac{1}{50})HCO_3^- + (\frac{fs}{20} - \frac{1}{50})NH_4^+ \mapsto \frac{fe}{10}N_2 + (\frac{4}{25} - \frac{3fs}{20})H_2O + \frac{fs}{20}C_5H_7C$$

2.2 NITRIFIER (AEROBIC REACTOR):

Parameter	*Nitrosomonas*	*Nitrobacters*	Aerobic Heterotrophs
f_s^0	0.14	0.10	0.7
Y	0.33 mgVSSa/mgNH$_4$	0.083mgVSSa/mgNO2	0.45mgVSSa/mgBOD$_L$
$\hat{q}$	1.7mgNH$_4$/mgVSSa-d	7.3 mgNO$_2$/mgVSSa-d	10mgBOD$_L$/mgVSSa-d
$\hat{q}$ mgO$_2$/mgVSSa-d	5.1	7.5	
K	0.57mgNH$_4$/L	0.62 mgNO$_2$/L	10 mgBOD$_L$/L
K_{Ox} mgO$_2$/L	0.5	0.68	
b d	0.082	0.082	0.1
$\left[\theta_x^{min}\right]_{lim}$ d	2.1	1.9	
$S_{min,Ox}$ mgO$_2$/L	0.084	0.12	
$S_{min,N}$	0.094 mgNH$_4$/L	0.1 mgNO$_2$/L	
f_d	0.067	0.067	0.8

Table 2: Typical parameters for a Nitrifier: T=15^{0}C (Table 9.1, p 472, Rittman and McCarty)

Nitrosomonas

$$R_a : \frac{1}{4}O_2 + H^+ + e^- \mapsto \frac{1}{2}H_2O$$

$$R_c : \frac{1}{5}CO_2 + \frac{1}{20}HCO_3^- + \frac{1}{20}NH_4^+ + H^+ + e^- \mapsto \frac{1}{20}C_5H_7O_2N + \frac{9}{20}H_2O$$

$$R_d : \frac{1}{6}NH_4^+ + \frac{1}{3}H_2O + e^- \mapsto \frac{1}{6}NO_2^- + \frac{4}{3}H^+$$

$$R : \frac{(1-fs)}{4}O_2 + \frac{fs}{5}CO_2 + \frac{fs}{20}HCO_3^- + (\frac{1}{6} + \frac{fs}{20})NH_4^+ \mapsto \frac{fs}{20}C_5H_7O_2N + \frac{1}{6}NO_2^- + (\frac{1}{6} - \frac{fs}{20})H_2O + \frac{1}{3}H^+$$

Nitrobacter:

$$R_a : \tfrac{1}{4}O_2 + H^+ \mapsto \tfrac{1}{2}H_2O$$

$$R_c : \tfrac{1}{5}CO_2 + \tfrac{1}{20}HCO_3^- + \tfrac{1}{20}NH_4^+ + H^+ \mapsto \tfrac{1}{20}C_5H_7O_2N + \tfrac{9}{20}H_2O$$

$$R_d : \tfrac{1}{2}NO_2^- + \tfrac{1}{2}H_2O \mapsto \tfrac{1}{2}NO_3^- + H^+$$

$$R : \tfrac{1-fs}{4}O_2 + H^+ + \tfrac{fs}{5}CO_2 + \tfrac{fs}{20}HCO_3^- + \tfrac{fs}{20}NH_4^+ + \tfrac{1}{2}NO_2^- \mapsto \tfrac{1}{2}NO_3^- \tfrac{fs}{20}C_5H_7O_2N + \tfrac{fs}{20}H_2O$$

Aerobic Heterotrophs:

$$R_a : \tfrac{1}{4}O_2 + H^+ \mapsto \tfrac{1}{2}H_2O$$

$$R_c : \tfrac{1}{5}CO_2 + \tfrac{1}{20}HCO_3^- + \tfrac{1}{20}NH_4^+ + H^+ \mapsto \tfrac{1}{20}C_5H_7O_2N + \tfrac{9}{20}H_2O$$

$$R_d : \tfrac{1}{50}C_{10}H_{19}O_3N + \tfrac{9}{25}H_2O \mapsto \tfrac{9}{50}CO_2 + \tfrac{1}{50}HCO_3^- + \tfrac{1}{50}NH_4^+ + H^+$$

$$R : \tfrac{1-fs}{4}O_2 + \tfrac{1}{50}C_{10}H_{19}O_3N + (\tfrac{fs}{5} - \tfrac{9}{50})CO_2 + (\tfrac{fs}{20} - \tfrac{1}{50})HCO_3^- + (\tfrac{fs}{20} - \tfrac{1}{50})NH_4^+ \mapsto \tfrac{fs}{20}C_5H_7O_2N + (\tfrac{7}{50} - \tfrac{fs}{20})H_2O$$

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), ρQ_2 (L/d), ν (1-ρ) Q2 (L/d). Input biochemical oxygen demands (BOD_L) are the carbon source, S^0 (mg BOD_L/L), the nitrogen (total Kjedahl nitrogen or TKN) source, Sn^0 (mg N/L), the nitrate-ion, *Sno* (mg NO3-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

$$
\begin{aligned}
&\text{biomass}: V_D \frac{dx_{P1}}{dt} = Q^0 x_P^0 + Q_2 f_d(\rho x_{v2} + \nu(1-\rho))x_w - Q_1 x_{p1} + \left(Y_P r_P - b_P x_{P1}\right)V_D \\
&\text{orgC}: V_D \frac{dS_1}{dt} = Q^0 S^0 + \rho Q_2 S_2 + \nu(1-\rho)Q_2 S_2 - Q_1 S_1 - r_P V_D \\
&\text{NO}_3^- : V_D \frac{dSno_1}{dt} = \rho Q_2 Sno_2 + \nu(1-\rho)Sno_2 - Q_1 Sno_1 - r_{no} V_D \\
&\text{TKN}: V_D \frac{dSnh_1}{dt} = Q^0 Sn^0 + \rho Q_2 Snh_2 + \nu(1-\rho)Q_2 Snh_2 - Q_1 Snh_1 - r_{nh} V_D \\
&\text{inerts}: V_D \frac{dx_{i1}}{dt} = Q^0 x_i^0 - Q_1 x_{i1} + (1-f_d)b(x_{v2} + x_w + x_{P1})V_D \\
&\text{utilRate}: r_P = \frac{\hat{q}_P S_1}{K_P + S_1} x_{P1} (\text{mgBOD}_L/\text{L - d})
\end{aligned}
\tag{4}
$$

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, $\hat{q}_P$ is the maximum specific rate of substrate utilization, b_P: is the endogenous decay coefficient, ρ is that fraction of the effluent stream (Q_2) of the nitrifier that is recycled to the denitrifier, Snh 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), θ_D, in the denitrifier, and the nitrifier, θ_N, respectively by

$$
\theta_D = \frac{V_D}{Q^0} \text{ and } \theta_N = \frac{V_N}{Q_1} \tag{5}
$$

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

$$
\theta_{xD} = \frac{V \cdot \text{active biomass}}{Q_1 \cdot \text{produced biomass}} \tag{6}
$$

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

$$
\theta = \frac{\theta_x}{w_v}\left(\frac{\Delta(V x_v)}{\Delta t}\right) = \lim_{t \to 0} \frac{\theta_x}{w_v}\left(\frac{d(V x_v)}{dt}\right) = \frac{\theta_x}{w_v}(Q_1 x_v) \tag{7}
$$

where w_v (mgVSSa/L) is the mixed-liquor volatile suspended solids (MLVSS or holdup) and $Q_1 x_v$ 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 $x_p^0 = 0$.
2. There are no TKN and organic carbons present in the effluent stream of the nitrifier. Thus, Snh_2=0, S_2=0.
3. There is no nitrate-ion in the effluent stream of the settler, thus Sno_e=0 but Sno_w =Sno_2.
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,

$$\begin{aligned}
\frac{dx_{P1}}{dt} &= \frac{Q_2}{V_D} f_d\left(\rho x_{v2} + \nu(1-\rho)x_w\right) - \frac{Q_1}{V_D} x_{P1} + \left(Y_P r_P - b_P x_{P1}\right) \\
\frac{dS_1}{dt} &= \frac{S^0}{\theta_D} - \frac{Q_1}{V_D} S_1 - r_P \\
\frac{dSno_1}{dt} &= \frac{Q_2}{V_D}\left(\rho + \nu(1-\rho)\right)Sno_2 - \frac{Q_1}{V_D} Sno_1 - r_{no} \qquad (8) \\
\frac{dSnh_1}{dt} &= \frac{Sn^0}{\theta_D} - \frac{Q_1}{V_D} Snh_1 - r_{nh} \\
\frac{dx_{i1}}{dt} &= \frac{x_i^0}{\theta_D} - \frac{Q_1}{V_D} x_{i1} + (1-f_d)b(x_{v2} + x_w + x_{P1})
\end{aligned}$$

Design variables are recycle fractions (ρ, ν), mean cell retention time, θ_{xD}, MLVSS, w_{vD}, Q_1, Q^0. Reasonable choices of ρ,$(1-\nu)(1-\rho)$ 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 (Sno_2) in stream 2 (effluent from nitrifier) that is an input stream to the denitrifier. Define

$$\gamma = \frac{14\,\text{mgN}}{113\,\text{mgVSS}} \qquad (9)$$

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,

$$\begin{aligned}
Q_2 Sno_2\,(\text{mgNO3/d}) &= Q^0 Sn^0 - \left(Q_1 x_{v1}^a + Q_2 x_{v2}^a\right)\gamma \\
x_{v1}^a &= x_{P1} + x_{i1} - x_i^0 \qquad (10) \\
x_{v2}^a &= x_{H2} + x_{N2} + x_{i2} - x_i^0
\end{aligned}$$

The dynamic balance is given by,

$$V_N \frac{dSno_2}{dt} = Q^0 Sn^0 - Q_1 x_{vD} \gamma - Q_2 Sno_2 - (r_N - r_H) V_N \qquad (11)$$

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,

$$\bar{S}nh_1 = \frac{(\frac{f_s}{20} - \frac{1}{50})}{50} (\frac{14\,\text{mgN}}{201\,\text{mgBOD}_L}) \text{ (substrate consumption rate)} \qquad (12)$$

3. The utilization, r_H, of the organic substrate, $C_{10}H_{19}O_3N$, 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:

$$\frac{\Delta(V_D x_{vD})}{\Delta t} (\text{mgVSS/d}) = Q_1 x_v = \frac{w_v Q^0 \theta_D}{\theta_{xD}} = \frac{w_v V_D}{\theta_{xD}} \qquad (13)$$

3.1.3 STEADY STATE

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

$$\bar{x}_{P1} = \left(\frac{Q_2}{V_D} f_d (\rho \bar{x}_{v2} + (1-\nu)(1-\rho)) \bar{x}_w - Y_P (\frac{S^0}{\theta_D} - \frac{Q_1 \bar{S}_1}{V_D}) \right) \frac{V_D}{Q_1 + b_P V_D}$$

$$\bar{S}_1 = \frac{-(\frac{Q^0 S^0}{Q_1} - K_P - \bar{q}_P \bar{x}_{P1} \frac{V_D}{Q_1}) \pm \sqrt{(\frac{Q^0 S^0}{Q_1} - K_P - \bar{q}_P \bar{x}_{P1} \frac{V_D}{Q_1})^2 - 4 \frac{Q^0 S^0 K_P}{Q_1}}}{2}$$

$$\bar{S}no_1 = \frac{-(\frac{Q_2}{Q_1} \bar{S}no_2 - K_{no} - \bar{q}_{no} \bar{x}_{P1} \frac{V_D}{Q_1}) \pm \sqrt{(\frac{Q_2}{Q_1} \alpha \bar{S}no_2 - K_{no} - \bar{q}_{no} \bar{x}_{P1} \frac{V_D}{Q_1})^2 - 4\alpha \frac{Q_2 \bar{S}no_2 K_{no}}{Q_1}}}{2} \qquad (14)$$

$$\alpha = (\rho + \nu(1-\rho))$$

$$\bar{S}nh_1 = \frac{-(\frac{Q^0}{Q_1} Sn^0 - K_{nh} - \bar{q}_{nh} \bar{x}_{P1} \frac{V_D}{Q_1}) \pm \sqrt{(\frac{Q^0}{Q_1} Sn^0 - K_{nh} + \bar{q}_{nh} \bar{x}_{P1} \frac{V_D}{Q_1})^2 - 4 \frac{Q^0 Sn^0 K_{nh}}{Q_1}}}{2}$$

$$\bar{x}_{i1} = \frac{V_D}{Q_1} \left(\frac{x_i^0}{\theta_D} + (1 - f_d) b_P (\bar{x}_{v2} + \bar{x}_{vw} + \bar{x}_{P1}) \right)$$

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

$$
\begin{aligned}
V_N \frac{dx_{H2}}{dt} &= Q_1 x_H^0 - Q_2 x_{H2} + (Y_H r_H - b_H x_{H2}) V_N \\
V_N \frac{dS_2}{dt} &= Q_1 S_1 - Q_2 S_2 - r_H V_N \\
V_N \frac{dx_{S2}}{dt} &= Q_1 x_{S1} - Q_2 x_{S2} + (Y_S r_S - b_S x_S) V_N \\
V_N \frac{dSnh_2}{dt} &= Q_1 Snh_1 - Q_2 Snh_2 - V_N r_S \\
V_N \frac{dx_{B2}}{dt} &= Q_1 x_{B1} - Q_2 x_{B2} + (Y_B r_B - b_B x_{B2}) V_N \\
V_N \frac{dSno2_2}{dt} &= Q_1 Sn_1 - Q_2 Sno2_2 - V_N r_B \\
V_N \frac{dx_{i2}}{dt} &= Q_0 x_i^0 - Q_2 x_{i2} + (1 - f_d)(b_H x_{H2} + b_N x_{N2} + b_B x_{B2}) V_N
\end{aligned}
\tag{15}
$$

The utilization terms r_H, r_S, and r_B are given by:

$$
\begin{aligned}
r_H &= \frac{\hat{q}_H S_2}{K_H + S_2} x_{H2} \\
r_S &= \frac{\hat{q}_S Snh_2}{K_S + Snh_2} x_S \\
r_B &= \frac{\hat{q}_B Sno2_2}{K_B + Sno2_2} x_{B2}
\end{aligned}
\tag{16}
$$

The total sludge leaving the denitrifier is given by:

$$
\frac{\Delta(V_N x_{vN})}{\Delta t}(\text{mgVSS/d}) = Q_2 x_v = \frac{w_{vN} Q_1 \theta_N}{\theta_{xN}} = \frac{w_v V_N}{\theta_{xN}} \tag{17}
$$

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*.

$$V_N \frac{dSno2_2}{dt} = Q_1\left(Sn_1 - \frac{\theta_N}{\theta_{xN}}(\bar{x}_H + \bar{x}_S + \bar{x}_i)\right)\gamma - Q_2 Sno2_2 - V_N r_B \qquad (18)$$

The amount of unused nitrogen is given by

$$\bar{S}n_2 = \bar{S}n_1 - \frac{\theta_N}{\theta_{xN}}(\bar{x}_a + \bar{x}_S + \bar{x}_B + \bar{x}_i)\gamma - \bar{S}nh_1 - \bar{S}no2_2 \qquad (19)$$

3.2.2 STEADY STATE

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

$$\begin{aligned}
\bar{x}_H &= \frac{\theta_{xN}}{\theta_N}\left(\frac{\bar{S}_1 - \bar{S}_2}{1 + b_H\theta_{xN}}\right)Y_H \\
\bar{S}_2 &= \frac{K_H(1 + b_H\theta_{xN})}{\theta_{xN}(Y_H\hat{q}_H - b_H) - 1} \\
\bar{x}_S &= \frac{\theta_{xN}}{\theta_N}\left(\frac{Snh_1 - \bar{S}nh_2}{1 + b_S\theta_{xN}}\right)Y_S \\
\bar{S}nh_2 &= K_S\frac{(1 + b_S\theta_{xN})}{\theta_{xN}(Y_S\hat{q}_S - b_S) - 1} \\
\bar{x}_B &= \frac{\theta_{xN}}{\theta_N}\left(\frac{\bar{S}no2_1 - \bar{S}no2_2}{1 + b_B\theta_{xN}}\right)Y_B \\
\bar{S}no2_2 &= K_B\frac{(1 + b_B\theta_{xN})}{\theta_{xN}(Y_B\hat{q}_B - b_B) - 1} \\
\bar{x}_{i2} &= \frac{\theta_{xN}}{\theta_N}\left(x_{i1}^0 + \theta_N(1 - f_d)(b_H\bar{x}_H + b_S\bar{x}_S + b_B\bar{x}_B\right)
\end{aligned} \qquad (20)$$

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

$$\frac{dV_T}{dt} = (1-\rho)Q_2 - (Q_e + Q_w) - (1-\nu)(1-\rho)Q_2$$

$$V_T \frac{dSno2_e}{dt} = (1-\rho)Q_2 Sno2_2 - (Q_e + Q_w + (1-\nu)(1-\rho)Q_2)Sno2_e \qquad (21)$$

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

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

$$\begin{aligned} Q_e + Q_w &= \nu(1-\rho)Q_2 \\ Sno2_e &= Sno2_2 \qquad (22) \\ x_{vw} &= \frac{(1-\rho)}{(1-\nu)(1-\rho)Q_2 + Q_w} Q_2 \end{aligned}$$

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

BAP	Biomass associated products
BOD	Biochemical oxygen demand
COD	Chemical oxygen demand
$C_{10}H_{19}O_3N$	Organic carbon substrate
$C_5H_7O_2N$	Cell or biomass empirical formula
HDT	Hydraulic detention time
MCRT	Mean cell retention time
MLVSS	Mixed liquor volatile suspended solids, mgVSS/L
OD	Oxygen demand (oxygen equivalents)
SMP	Soluble microbial products
SRT	Solids retention time
TKN	Total Kjeldahl nitrogen
UAP	Utilization associated products
VSS,VSSa	Volatile suspended solids, active volatile suspended solids
b	Endogenous rate of decay coefficient, 1/d
d	Day
f_e	Fraction of electrons used for energy
f_d	Fraction of active biomass that is biodegradable
f_s	Fraction of electrons used for synthesis
f_s^0	Total number of electrons transferred to the electron acceptor
r_k	Rate of utilization by biomass component K (K=B,H,P,S)
K	Substrate concentration that give ½ the maximum rate, mgBOD$_L$/L
$\hat{q}$	Maximum specific rate of substrate utilization, mgBOD$_L$/mgVSS-d
Q^0	Inlet volumetric feed rate, L/d
Q_j	Volumetric rate of stream j, L/d
r	Rate of substrate utilization, mgBOD$_L$/L-d
R_e	Energy reaction
R_d	Donor reaction
R_s	Cell synthesis reaction
S^0	Organic substrate influent concentration, mgBOD$_L$/L
S_j	Substrate concentration in stream j, mgBOD$_L$/L
Sno	Nitrate-ion concentration, mgNO3-N/L
$Sno2$	Nitrite-ion concentration, mgNO2-N/L
Snh	Ammonium concentration, mgNH4-N/L
Sn^0	Influent nitrogen concentration mgN/L
x_{kj}	kth biomass component in stream j, mgVSSa/L
x_i^0	Influent inert concentration, mgVSS/L
x_{vj}^a	Active volatile suspended solids in stream j, mgVSS/L
x_i	Non-biodegradable portion of the biomass, mgVSS/L
x_B	Concentration of biomass associated products, mgBOD/L
x_U	Concentration of utilized associated products, mgBOD/L
V_D, V_N, V_T	Denitrifier volume, nitrifier volume, settler volume, L/d

Y	True cell synthesis yield, mgVSS/mgBOD_L
Y_n	Net yield, mgVSS/mgBOD_L

GREEK LETTERS

ρ	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
γ	Ratio of ½ molecular weight of nitrogen to that of biomass
θ_D, θ_N	Hydraulic detention time (HDT) in denitrifier and nitrifier, d
θ_x	Mean cell retention time (MCRT) or solids retention time (SRT), d
$\theta_{x,min}$	Min MCRT) or min SRT, d
$[\theta_{x,min}]_{lim}$	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

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