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Model Development and Simulation of Nitrification in SHARON Reactor in Moderate Temperature by Simulink

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ABSTRACT : *In order to reduce the nitrogen compounds in WWTP effluent according to legislations, nitrogen of reject water is removed in separate unit by applying innovative cost effective process named SHARON (Single reactor High activity Ammonium Removal Over Nitrite) process which is feasible to apply in moderate weather and more cost effective process due to elimination the heat exchanger required to keep the reject water of high temperature. In addition to the save in oxygen requirement to oxide ammonium by preventing nitrite oxidation and the saving in external COD addition for denitrification. Also, there is no need for large reactor volume because HRT equal to SRT. Significant mathematical model of nitrification process in SHARON reactor was developed based on substances and organisms mass balance as well as organisms kinetics. A relatively favorable consistency was obtained between the experimental and the predicted results of model. A high correlation of (R^2=0.946) between model predictions and experimental data sets.*

KEYWORDS : *SHARON, nitrification, model, moderate temperature.*

I. INTRODUCTION

The presence of nitrogen compounds is a significant problem in wastewater treatment process. It is difficult to obtain and maintain sufficient nitrifiers in wastewater treatment plants with short sludge retention time (SRT) [12]. Because the nitrifiers growth is slow due to effects of environment change in biological reactor such as toxic shock and pH [3]. For nitrification design in conventional activated sludge processes safety factor is used to get long SRT to increases the concentration of mixed liquor suspended solids (MLSS) which requires large and clarifiers tanks and other sludge conditioning units to accommodate the accumulation of solids [11]. High nitrogen wastewater is typically generated in reject water (side stream wastewater) such as anaerobic sludge digestion and drying bed filtrates. During sludge treating before final disposal to reduce the volume of sludge by removal of water, which constitutes 97-98% of sludge and to reduce the volatile content to eliminate the harm and threat to human health, the nitrogen is fraction in the organic matter is converted to soluble ammonia. The reject water from dewatering of hydrolyzed sludge has high ammonium content, typically 500-1500 *mg/l* and it is 20-30 times stronger than that of influent [14]. Reject water recycling to the main stream of wastewater treatment plant increase the total nitrogen load with 15-20% [6,13], but because the flows are relatively low, they are about 1% of the main line, cost effective nitrogen removal in small reactors can be achieved [9]. Among the possible treatment options are SHARON process(Single reactor system for High activity Ammonium Removal Over Nitrite). The aim of a mathematical model during simulation is to describe the performance of SHARON process. Thus, a model can contribute for better understanding of process operation and kinetics. There were two types of models were combined to described the process; 1) mass balance model that described mass transport in SHARON reactor; 2) and kinetic model which described the growth rate of ammonium oxidizing organism and nitrite oxidizing organism depend on the reactor conditions. The equations described mass balance in well mixed bioreactor for unsteady state was ordinary differential equations. The growth of ammonium oxidizer organism and nitrite oxidizer organism was associated with dissolved oxygen consumption , pH variation and temperature variation.

II. NITRIFICATION MODEL

The proposed mathematical model focuses on the prediction of the substrates removal and microorganism growth in the system. The model had to be able to predict the change of DO and pH. The main process parameters include oxygen concentration, temperature and HRT The model considers two substrates, ammonium and nitrite, and two groups of microorganisms, ammonium oxidizers and nitrite oxidizers were taking into account. The SHARON reactor is continuous stirred tank reactor (CSTR) and consists liquid and gas phases were made to facilitate the numerical solution of the model. In addition, quantitative and qualitative uniform istribution of organisms and substrates in the reactor was considered and interphase transport of oxygen is considered. The model assumed that the feed stream does not contain any ammonium oxidizer or nitrite oxidizer organisms.The ammonium consider available with high concentration which sufficient for growth process.

III. MATERIAL BALANCES

Based on equations (1-6), the equilibrium reactions considered as follows:
The stoichiometric reaction for oxidation of ammounium to nitrite:

$$NH_4^+ + 1.5O_2 \rightarrow 2H^+ + H_2O + NO_2^- \quad \text{..... (1)}$$

The stoichiometric reaction for oxidation of nitrite to nitrate:

$$NO_2^- + 0.5O_2 \rightarrow NO_3^- \quad \text{..... (2)}$$

All the reactions take place in aquatic system in which the carbonic acid bicarbonate equilibrium take place according the following :

$$H_2O + CO_2 \longleftrightarrow H_2CO_3 \longleftrightarrow H^+ + HCO_3^{-+} \quad \text{..... (3)}$$

Representing the bacterial composition as ($C_5H_7NO_2$) and by combining equation (1) and (2) with equation (3)yield the following equations:

$$NH_4^+ + 1.5O_2 + 2HCO_3^- \rightarrow NO_2^- + 2H_2CO_3 + H_2O + 58{\sim}84\ Kcal \quad \text{..... (4)}$$

$$13NH_4^+ + 23\ HCO_3^- \rightarrow 8\ H_2CO_3 + 10\ NO_2^- + 3\ C_5H_7NO_2 + 19\ H_2O \quad \text{.....(5)}$$

$$NH_4^+ + 10\ NO_2^- + 4\ H_2CO_3 + HCO_3^- \rightarrow 10\ NO_3^- + 3\ H_2O + 3\ C_5H_7NO_2 \quad \text{.....(6)}$$

The dynamic model, which consists of four differential equations, is based on substrate and organism mass balances around the reactor. For continuous flow, continuous stirred tank reactor (CSTR) the general equation for the substrate material balance may be expressed as below:

$$Accumulation = In - Out + Generation \quad \text{.....(7)}$$

The same expression can be applied for organism material balance. In the differential equations, all the terms associated with ammonium, nitrite and nitrate concentrations are expressed as *mg/l* of N.
The mass balance of ammonium nitrogen is:

$$\frac{dS_1^{NH3}}{dt} = \frac{Q}{V}\left(S_0^{NH3} - S_1^{NH3}\right) - \mu^{am}\frac{X_1^{am}}{Y^{am}} \quad \text{.....(8)}$$

The mass balance of nitrate nitrogen can be written as:

$$\frac{dS_1^{NO2}}{dt} = \frac{Q}{V}\left(S_0^{NO2} - S_1^{NO2}\right) - \mu^{nit}\frac{\mu_1^{nit}}{Y^{nit}} \quad \text{.....(9)}$$

The oxygen transfer from gas phase to liquid follow the two films theory for gas transfer, which assume the gas – liquid interface include gas film and liquid film through which the gas is transfer by molecular diffusion. The diffusion in the liquid phase is usually the control for overall rate of mass transfer because of much lower diffusivity in this phase. Also, the gas film thickness is much smaller than liquid film thickness because mobility of molecular in gas phase is much greater than liquid phase. The net transfer from the gas phase to the liquid phase is given by:

$$\frac{dS_{O2}^{liquid}}{dt} = ka\left(S_{O2}^{sat} - S_{O2}^{liquid}\right) \quad . \quad \text{....(10)}$$

Henry's law which states "the weight of gas that can be dissolved in given volume of liquid is directly proportional to the pressure that the gas exerts above the liquid" assumed to apply at the interface to calculate the saturation concentration of oxygen in wastewater as below [5]:

$$S_{O2}^{sat} = K_H P_{O2} \quad \text{.....(11)}$$

The saturation concentration of oxygen in wastewater will be different from that of fresh water as:

$$S_{wO2}^{sat} = \beta S_{O2}^{sat} \qquad \text{.....(12)}$$

Whereβ =0.8. The mass transfer coefficient of oxygen expressed in (d^{-1}), is related to superficial gas velocity which expressed in (*m/s*). for air water bubble columns with coarse bubble, the linear relationship can be used [16]:

$$ka = 0.6\, U_g \qquad \text{.....(13)}$$

According [1], the superficial gas velocity can be taken as (*0.02m/s*). the mass transfer coefficient varies with temperature according Arrhenius equation as below:

$$ka_T = ka\ \theta^{(T-20)} \qquad \text{.....(14)}$$

The common value of reported is 1.024 for mechanical and diffused aeration device [10].

Based on equations (11) to (14), equation (10) can be written as:

$$\frac{dS_{O2}^{liquid}}{dt} = 0.6\, U_g\, \theta^{(T-20)}\left(\beta S_{O2}^{sat} - S_{O2}^{liquid}\right) \qquad \text{.....(15)}$$

Based on equation (1), the stoichiometric requirement of oxygen for ammonium oxidation is 3.43 mg of O_2 per mg of *NH4-N* [11]. The oxygen utilization term for the oxidation of ammonium per unit volume of reactor per unit time is:

$$O_{2_{consumed}} = 3.43\ \times oxidation\ rate\ of\ NH_4^+ asN \qquad \text{.....(16)}$$

Where, $oxidation\ rate\ of\ NH_4^+ asN = \mu^{am}\frac{x_1^{am}}{\gamma^{am}}\ asN$ .....(17)

The oxygen balance in liquid for nitrification phase of SHARON reactor can be written as:

$$\frac{dS_{O2}^{liquid}}{dt} = 0.6\, U_g\, \theta^{(T-20)}\left(\beta S_{O2}^{sat} - S_{O2}^{liquid}\right) - 3.43\mu^{am}\frac{x_1^{am}}{\gamma^{am}}\ (mg/l.sec) \qquad \text{.....(18)}$$

Organisms balances

The mass balances of the ammonium oxidizer and nitrite oxidizer organisms around the reactor can be expressed as:

$$\frac{dx_1^{am}}{dt} = \frac{Q}{\forall}\left(X_0^{am} - X_1^{am}\right) + \mu^{am}.X_1^{am} \qquad \text{.....(19)}$$

$$\frac{dx_1^{nit}}{dt} = \frac{Q}{\forall}\left(X_0^{nit} - X_1^{nit}\right) + \mu^{nit}.X_1^{nit} \qquad \text{.....(20)}$$

Since the feed stream does not contain any ammonium oxidizer or nitrite oxidizer organisms.
So, the equations (19) and (20) can be written as:

$$\frac{dx_1^{am}}{dt} = -\frac{Q}{\forall}X_1^{am} + \mu^{am}.X_1^{am} \qquad \text{.....(21)}$$

$$\frac{dx_1^{nit}}{dt} = -\frac{Q}{\forall}X_1^{nit} + \mu^{nit}.X_1^{nit} \qquad \text{.....(22)}$$

IV. ESTIMATION OF GROWTH RATES OF NITRIFICATION ORGANISM

All biochemical experiments carry out previously on different organism culture indicate that the kinetics are influenced by many factors such as substrate concentration, product concentration, pH, temperature, dissolved oxygen and various inhibitors. The specific growth rate is commonly expressed by multiplication of Monod type expressions of each individual term. According [15,16], the specific growth rate coefficient for mmonium oxidizer and nitrite oxidizer can be expressed as:

$$\mu^{am} = \mu^{am}_{max} \cdot \frac{S_1^{NH_3}}{K^{am}_{NH_3} + S_1^{NH_3}} \cdot \frac{S_1^{O_2}}{K^{am}_{O_2} + S_1^{O2}} \quad .....(23)$$

$$\mu^{nit} = \mu^{nit}_{max} \cdot \frac{S_1^{NO2}}{K^{nit}_{NO2} + S_1^{NO2}} \cdot \frac{S_1^{O_2}}{K^{nit}_{O_2} + S_1^{O2}} \quad .....(24)$$

The temperature dependency of maximum specific growth rates of ammonium oxidizer organism and nitrite oxidizer organism was taking into account using the Arrhenius equation:

$$\mu_T = \mu_{20} e^{\theta(T - T_r)} \quad .....(25)$$

The dependence of maximum specific growth rates of ammonium oxidizer organism and nitrite oxidizer organism was modeled using the relationship of Van Hulle et al.; 2007 [16]:

$$OUR = OUR_{max} \frac{K_{pH}}{K_{pH} - 1 + 10^{\left(pH_{opt} - pH\right)}} \quad .....(26)$$

Where, K_{pH} = 8.21 and pH_{opt} = 7.23. Equation (26), is applied here for maximum specific growth rates of ammonium oxidizer organism and nitrite oxidizer organism instead of oxygen uptake rate (*OUR*).

$$\mu = \mu_{max} \frac{K_{pH}}{K_{pH} - 1 + 10^{\left(pH_{opt} - pH\right)}} \quad .....(27)$$

Based on the above considerations, the following expressions for the specific growth rate of ammonium and nitrite oxidizes organisms are proposed:

$$\mu^{am} = \mu^{am}_{max} \cdot \frac{S_1^{NH_3}}{K^{am}_{NH_3} + S_1^{NH_3}} \cdot \frac{S_1^{O_2}}{K^{am}_{O_2} + S_1^{O2}} \cdot \frac{K_{pH}}{K_{pH} - 1 + 10^{\left(pH_{opt} - pH\right)}} \cdot e^{\theta(T-20)} \quad .....(28)$$

$$\mu^{nit} = \mu^{nit}_{max} \cdot \frac{S_1^{NO2}}{K^{nit}_{HNO2} + S_1^{NO2}} \cdot \frac{S_1^{O_2}}{K^{nit}_{O_2} + S_1^{O2}} \cdot \frac{K_{pH}}{K_{pH} - 1 + 10^{\left(pH_{opt} - pH\right)}} \cdot e^{\theta(T-20)} \quad .....(29)$$

The values of parameters was used in the model were selected by literature survey and presented in Table (1) . The specific yield value used were 0.15 *mg* NH_4^+*-N/L* for ammonia oxidizer [2].

V. RESULTS

A simulink which is graphical extension to MATLAB program version 7.11.0.584(R2010b) was applied to solve the set of equations suggested for the developed model.The implementation of SHARON process in Simulink model has been shown in Figure (1).

Model predictions : The kinetics parameters and constants related to the performance of SHARON process Table (1) were characterized and adopted to develop a theoretical relationship of variation for the substrate concentration (ammonium and nitrite). The yield coefficient as well as the dilution rate and the experimental influent concentration of ammonium were experimentally determined.

The variation of ammonium, nitrite, and nitrate are given in Figure (2). The variation of DO concentration during aerobic phase of SHARON process taking in account the saturation DO concentration for water of temperature 27.48 ℃ which represent the average temperature during operation of lab scale SHARON reactor experiment to simulate the weather condition is given in Figure (3).

Comparison of model predictions and experimental results : Comparisons between the predicated result and experimental results shown in Figure (4). In general, the model predictions significantly and successfully agree with the experimental data sets. A reasonable agreement between the predicated results and experimental results can be recognized. Overall, the model predictions successfully show a very good correlation (R^2=0.946) with the experimental data sets. The slight variations between the model predictions and experimental results may be attributed to the simplifications and assumptions made in the developed model such as (1) a uniform distribution of microbial populations in the reactor was assumed; (2) the influent ammonium is well distributed in the reactor; (3) constant reactor temperature and pH was assumed; (4) and no DO consumption by aerobic heterotrophic organism was assumed.

FIGURES AND TABLES

Table (1): the parameters as well as the constants used for the model development and imulation for nitritation of SHARON process model.

Parameter	Symbol	unit	Value	Reference
maximum specific growth rate of ammonia oxidizer	μ_{max}^{am}	d^{-1}	1.22	[7]
maximum specific growth rate of nitrite oxidizer	μ_{max}^{nit}	d^{-1}	0.02 to .17	[8]
ammonia substrate saturation for ammonia oxidizers	$K_{NH_3}^{am}$	mg/L	5.14	[4]
nitrite acid substrate saturation for nitrite oxidizers	K_{NO2}^{nit}	mg/L	0.27	[4]
oxygen substrate saturation for ammonia oxidizers	$K_{O_2}^{am}$	mg/L	0.23	[17]
oxygen substrate saturation for nitrite oxidizers	$K_{O_2}^{nit}$	mg/L	1.5	[17]
Arrhenius constant for ammonia oxidizers	θ	-	0.094	[17]
Arrhenius constant for nitrite oxidizers	θ	-	0.061	[17]

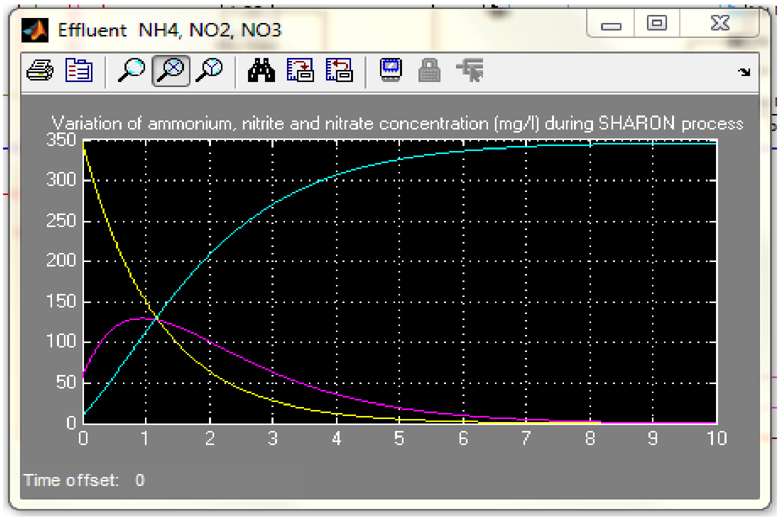

Figure (2): Simulink simulation of effluent ammonium (Yellow), nitrite (Cyan) and nitrate (Magenta) concentration during SHARON process operation

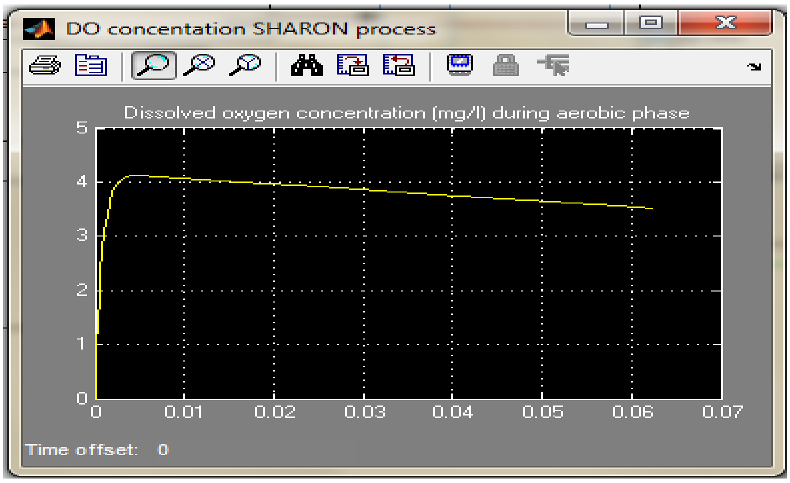

Figure (3): Simulink simulation of DO concentration for aerobic phase of SHARON process.

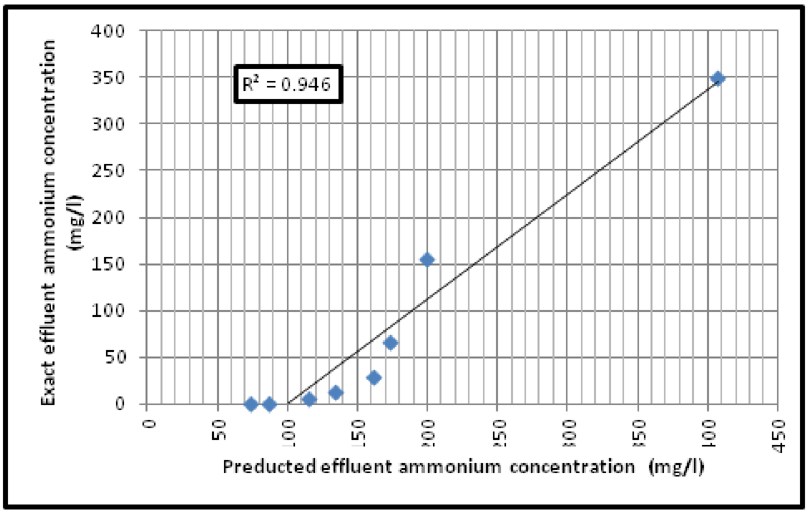

Figure (4): Correlation between exact and predicted by model of effluent ammonium concentration during SHARON process.

VI. CONCLUSION

Significant mathematical model of nitrification process in SHARON reactor was developed based on substances and organisms mass balance as well as organisms kinetics. A relatively favorable consistency was obtained between the experimental and the predicted results of model. A high correlation of (R^2=0.946) between model predictions and experimental data sets.

VII. NOMENCLATURE

S	substrate concentration (mg/L as N)	P_{O2}	partial pressure of O_2 (atm), determined by Dalton's law.
Q	flow rate (l/sec)	U_g	superficial gas velocity (m/s)
$\frac{Q}{\forall}$	dilution rate (d^{-1})	T	temperature °C
$\forall$	reactor volume (l)	θ	Arrhenius constant
X	organism concentration (mg/l)	K	substrate saturation coefficient (mg/l)
μ^{am}	ammonium oxidizer organism specific growth rate coefficient(d^{-1})	μ_T	maximum specific rate at real temperature

Y^{am}	yield coefficient of ammonium oxidizer coefficient	μ_{max}^{am}	maximum specific growth rate of ammonium oxidizer(d^{-1})
S_{O2}^{liquid}	concentration of oxygen gas in water (*mg/l*)	μ_{max}^{nit}	maximum specific growth rate of nitrite oxidizer(d^{-1})
ka	mass transfer coefficient	μ_{20}	maximum specific rate at reference temperature $=20°C$
S_{O2}^{sat}	saturation concentration of oxygen gas in water (*mg/l*)	θ	Arrhenius constant
K_H	Henry's law constant (*mg/l/atm*)	T_r	reference temperature (°C)

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